ReaxysFile™ on STN: Displaying REACH Relevant Data

Example 1: REACH relevant data for an organic substance (S <CAS RN>, D REACH)

Example 2: REACH relevant data for an inorganic substance (S <MF>, D REACH)

In 2007, the EU launched the REACH (Registration, Evaluation, Authorisation and Restriction of Chemicals) directive in order to establish a Europe-wide standard directive for producing and handling chemicals. This means that all companies producing and trading chemicals are required to collect and supply detailed data of their chemicals.

ReaxysFile helps you comply with these regulations by providing you with information on

- Structures of chemical compounds
- Chemistry and physics data
- Toxicological properties

A special display format which combines all relevant property fields that are required for the REACH process is available in ReaxysFile.

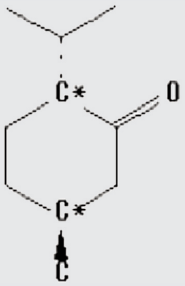
Included properties are:

- Melting Point (MP)
- Sublimation Point (SP)
- Boiling Point (BP)
- Vapor Pressure (VP)
- Optical Rotatory Power (ORP)
- Refractive Index (RI)
- Mutarotation (MUT)
- Liquid Density (DEN)
- Dissociation Exponent (DE)
- Solubility (SLB)
- Heat Capacity (CP)
- Heat Capacity (CV)
- Enthalpy of Formation (HFOR)
- Enthalpy of Vaporization (HVAP)
- Flash Point (FP)
- Ecological Data (ECO)
- Pharmacological Data (PHARM)

The price of this format is “query related”, which means all available display fields are charged.

Example 1: REACH relevant data for an organic substance (S <CAS RN>, D REACH)

```
  Accession Number (AN):              2041368
  Basic Pref. RN (BPR):               10458-14-7
  CAS Reg. No. (RN):                  10458-14-7, 14073-97-3
  Chemical Name (CN):                 L-menthone,
                                      (2S,5R)-2-isopropyl-5-methylcyclohexanone,
                                      (2S,5R)-menthone, L-(-)-menthone,
                                      (-)-Menthone, (-)menthone,
   (2S,5R)-5-Methyl-2-(1-methylethyl)cyclohex
                                      anone
  Autonom Name (AUN):                 (2S,5R)-2-Isopropyl-5-methyl-cyclohexanone
  Lin. Struct. Formula (LSF):         C9H18OC
  Molec. Formula (MF):                C10 H18 O
  Formula Weight (FW):                154.252
  Compound Type (CTYPE):              isocyclic
  InChi Key: (INCHI):                 NFLGAXVYCFJBMK-BDAKNGLRSA-N
  Alternate InChi Key: (AINCHI):      NFLGAXVYCFJBMK-BDAKNGLRBF
  Markush Ref. Count (MARKREF):       0
  Entry Date (DED):                   1989/06/29
  Update Date (DUPD):                 2011/03/20
```



Field Availability:

Code	Name	Occurrence
AN	Accession Number	1
BPR	Basic Preferred RN	1
RN	CAS Registry Number	2
CN	Chemical Name	7
AUN	Autonomname	1
LSF	Linearized Structure Formula	1
MF	Molecular Formula	1
FW	Formula Weight	1
INCHI	InChi Key	1
AINCHI	Alternate InChi Key	1
CTYPE	Compound Type	1
MARKREF	Markush Reference Count	1
DED	Entry Date	1
DUPD	Update Date	1
ADSM	Adsorption (MCS)	1
ASSM	Association (MCS)	23
AZE	Azeotrope (MCS)	3
BP	Boiling Point	19
CDER	Chemical Derivative	9
CDIC	Circular Dichroism	2
CNF	Conformation	2
CPD	Crystal Property Description	2
DEN	Density (Liquid)	8
DIC	Dielectric Constant	1
DM	Dipole Moment	5
DV	Dynamic Viscosity	1
ECTOX	Ecotoxicology	18
EXCA	Exposure Assessment	1
INP	Isolation from Natural Product	7
IR	Infrared Spectrum	11
LB	Substance Label	85
LLSM	Liquid/Liquid System (MCS)	2
LVSM	Liquid/Vapour System (MCS)	1
MP	Melting Point	3
MS	Mass Spectrum	3
NMR	Nuclear Magnetic Resonance	28

ORD	Optical Rotatory Dispersion	4
ORP	Optical Rotatory Power	39
PHARM	Pharmacological Data	21
RAS	Raman Spectrum	1
RI	Refractive Index	8
RSTR	Related Structure	1
SLB	Solubility (MCS)	6
ST	Surface Tension	2
USC	Use of Compound	3
UVS	UV and Visible Spectrum	8
XREF	Crossfile Reference	5

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1358
RX.RAN	Reactant AN	1237
RX.PAN	Product AN	121

Melting Point:

Value (MP) (Cel)	Ref.
-5.7	1
-6.55	2
-7	3

Reference(s):

1. Huggett, Journal of the Society of Chemical Industry, London, CODEN: JSCIAN, 60, <1941>, 67, Quarterly Journal of Pharmacy and Pharmacology, CODEN: QJPPAL, 15, <1942>, 218
2. Fischer, Bulletin des Societes Chimiques Belges, CODEN: BSCBAG, 49, <1940>, 129,133
3. Zeitschel; Schmidt, Chemische Berichte, CODEN: CHBEAM, 59, <1926>, 2303

Boiling Point:

Value (BP) (.P) (Cel)	Press. (Torr)	Ref.	Note
203 - 204	760	1	
102	20	2	
207 - 208	760	3	
207 - 209		4	
80 - 82	11	5	
70 - 72	1	6	
202 - 203	760	7	
88 - 93	14	8	
86 - 92	18	9	
65	4	10	
86 - 88	15	11	
208 - 211		12	
83 - 84	11	13	
118	41	14	
83 - 84	12	15	
83 - 84	9 - 10	16	
75 - 77	2	17	1
210	760	18	
210 - 210.25		19	

Reference(s):

1. Jain, Suman L.; Sharma, Vishal B.; Sain, Bir, Tetrahedron, CODEN: TETRAB, 62(29), <2006>, 6841 - 6847
2. Rajkumar, G. Abraham; Sivamurugan, V.; Arabindoo, Banumathi; Murugesan, V., Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry, CODEN: IJSBDB, 43(5), <2004>, 936 - 946
3. Mohajerani, Bagher; Heravi, Majid M.; Ajami, Dariush, Monatshefte fuer Chemie, CODEN: MOCMB7, 132(7), <2001>, 871 - 874
4. Lochynski, Stanislaw; Kuldo, Joanna; Frackowiak, Bozena; Holband, Jolanta; Wojcik, Grazyna, Tetrahedron: Asymmetry, CODEN: TASYE3, 11(6), <2000>, 1295 - 1302
5. Chen, Fener; Liu, Anchang; Yan, Qiongjiao; Liu, Mingxing; Zhang, Daoming; Shao, Lanying, Synthetic Communications, CODEN: SYNCAV, 29(6), <1999>, 1049 - 1056
6. Sato, Kazuhiko; Aoki, Masao; Takagi, Junko; Zimmermann, Klaus; Noyori, Ryoji, Bulletin of the Chemical Society of Japan, CODEN: BCSJA8, 72(10), <1999>, 2287 - 2306

7. Shaabani, Ahmad; Ameri, Majid, Journal of Chemical Research, Synopses, CODEN: JRPSDC(2), <1998>, 100 - 101
8. Jansen, Ursula; Runsink, Jan; Mattay, Jochen, Liebigs Annalen der Chemie, CODEN: LACHDL(3), <1991>, 283 - 285
9. Falorni, Massimo; Lardicci, Luciano; Uccello-Barretta, Gloria; Giacomelli, Giampaolo, Gazzetta Chimica Italiana, CODEN: GCITA9, 118(7), <1988>, 495 - 500
10. Duraisamy, M.; Walborsky, H. M., Journal of the American Chemical Society, CODEN: JACSAT, 105(10), <1983>, 3252 - 3264
11. Maslinska-Solich, Jolanta; Rudnicka, Irena; Jedlinski, Zbigniew J., Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999), CODEN: JCPRB4, <1981>, 3034 - 3040
12. Doleschall, Gabor; Toth, Gabor, Tetrahedron, CODEN: TETRAB, 36, <1980>, 1649 - 1666
13. Derdzinski,K.; Zabza,A., Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques, CODEN: BAPCAQ, 25, <1977>, 529 - 540
14. Shono,T. et al., Tetrahedron Letters, CODEN: TELEAY, <1974>, 1295 - 1298
15. Voisin; Gastambide, Bulletin de la Societe Chimique de France, CODEN: BSCFAS, <1971>, 2643,2650
16. Bell; Caldin, Journal of the Chemical Society, CODEN: JCSOA9, <1938>, 382,387, 389
17. Grignard; Savard, Bulletin des Societes Chimiques Belges, CODEN: BSCBAG, 36, <1927>, 106, Chem. Zentralbl., CODEN: CHZEA6, 98(I), <1927>, 2998
18. Zeitschel; Schmidt, Chemische Berichte, CODEN: CHBEAM, 59, <1926>, 2303
19. Wallach, Justus Liebigs Annalen der Chemie, CODEN: JLACBF, 437, <1924>, 193, Justus Liebigs Annalen der Chemie, CODEN: JLACBF, 414, <1918>, 332

Notes(s):
1. Enolform des Menthons, p-Menthen-(3)-ol-(3).

Optical Rotatory Power:

Part 1 of 2	Value (ORP) (deg)	Type (.TYP)	Concentr. (.C)	Length of Path (.LEN) (ORP) (cm)	Solvent (.SOL)	Ref.
1	-23.1	[alpha]	5.18 g/100ml		chloroform	1
2	-27.9	[alpha]	1 g/100ml		chloroform	2
3	-28.6	[alpha]	1.1 g/100ml		ethanol	3
4	-25.3	[alpha]			neat liquid	4
5	-31	[alpha]	1.0 g/100ml		CHCl3	5
6	-23	[alpha]			methanol	6
7	-30	[alpha]	1.0 g/100ml		methanol	7
8	-24.6	[alpha]			neat (no solvent)	8
9	-24	[alpha]				9
10	-24.6	[alpha]	4.55 g/100ml		methanol	10
11	-24.5	[alpha]				11
12	-28.5	[alpha]			neat (no solvent)	12
13	-24.5	[alpha]			neat (no solvent)	13
14	-29.3	[alpha]			neat (no solvent)	14
15	-25.7	[alpha]	1.1 g/100ml		ethanol	15
16	-27.3	[alpha]	1.0 g/100ml		ethanol	16, 17
17	-28.3	[alpha]				18, 19
18	-29.8	[alpha]				20
19	-29.5	[alpha]	2.0 g/100ml		CHCl3	21
20	-27.8	[alpha]		4	neat (no solvent)	22

Optical Rotatory Power:

Part 2 of 2	Wavelen. (.W) (nm)	Temp. (.T) (Cel)	Note	Ref.
1	589	20		1
2	589	25		2
3	589			3
4	589			4
5	589	25		5
6	589	20		6
7	589	20		7
8	580	20		8
9	589			9
10	589	23		10
11	589	24		11
12	589			12

13	589	24		13
14	589	25		14
15	589	25		15
16	589	25		16, 17
17	589	25		18, 19
18	589	20		20
19	589	27		21
20	589	25	1	22

Reference(s):

1. Tuktarov, Airat R.; Korolev, Vyacheslav V.; Tulyabaev, Artur R.; Popod'Ko, Natal'Ya R.; Khalilov, Leonard M.; Dzhemilev, Usein M., Tetrahedron Letters, CODEN: TELEAY, 52(7), <2011>, 834 - 836
2. Hodgson, David M.; Salik, Saifullah; Fox, David J., Journal of Organic Chemistry, CODEN: JOCEAH, 75(7), <2010>, 2157 - 2168
3. Timshina, A. V.; Rubtsova, S. A.; Kuchin, A. V.; Kodess, M. I.; Matochkina, E. G.; Slepukhin, P. A., Russian Journal of Organic Chemistry, CODEN: RJOCEQ, 44(7), <2008>, 1043 - 1048, Zhurnal Organicheskoi Khimii, CODEN: ZORKAE, 44(7), <2008>, 1053 - 1058
4. Barry, Conor S.; Bushby, Nick; Harding, John R.; Willis, Christine L., Organic Letters, CODEN: ORLEF7, 7(13), <2005>, 2683 - 2686
5. Nokami, Junzo; Ohga, Masanori; Nakamoto, Hitoshi; Matsubara, Tadahiro; Hussain, Iqbal; Kataoka, Kazuhide, Journal of the American Chemical Society, CODEN: JACSAT, 123(37), <2001>, 9168 - 9169
6. Lochynski, Stanislaw; Kuldo, Joanna; Frackowiak, Bozena; Holband, Jolanta; Wojcik, Grazyna, Tetrahedron: Asymmetry, CODEN: TASYE3, 11(6), <2000>, 1295 - 1302
7. Chen, Fener; Liu, Anchang; Yan, Qiongjiao; Liu, Mingxing; Zhang, Daoming; Shao, Lanying, Synthetic Communications, CODEN: SYNCAV, 29(6), <1999>, 1049 - 1056
8. Odinokov, V. N.; Botsman, L. P.; Emel'yanova, G. A., Russian Chemical Bulletin, CODEN: RCBUEY, 47(10), <1998>, 2021 - 2022, Izvestiya Akademi Nauk, Seriya Khimicheskaya, CODEN: IASKEA(10), <1998>, 2077 - 2078
9. Burgemeister, Thomas; Oezarslan, Oezdemir; Ertan, Mevluet; Akguen, Huelya; Wiegrebe, Wolfgang, Archiv der Pharmazie (Weinheim, Germany), CODEN: ARPMAS, 327(12), <1994>, 785 - 788
10. Hiroi, Kunio; Umemura, Masayuki, Tetrahedron, CODEN: TETRAB, 49(9), <1993>, 1831 - 1840
11. Odinokov, V. N.; Ishmuratov, G. Yu.; Yakovleva, M. P.; Safiullin, R. L.; Komissarov, V. D.; Tolstikov, G. A., Russian Chemical Bulletin, CODEN: RCBUEY, 42(7), <1993>, 1244 - 1245, Izvestiya Akademii Nauk SSSR, Seriya Khimicheskaya, CODEN: IASKA6(7), <1993>, 1301 - 1303
12. Adje, N.; Breuilles, P.; Uguen, D., Tetrahedron Letters, CODEN: TELEAY, 33(16), <1992>, 2151 - 2154
13. Odinokov, V. N.; Ishmuratov, G. Yu.; Yakovleva, M. P.; Muslukhov, R. R.; Safiullin, R. L.; et al., Doklady Chemistry, CODEN: DKCHAY, 326(4-6), <1992>, 231 - 235, Dokl. Akad. Nauk SSSR Ser. Khim., CODEN: DASKAJ, 326(5), <1992>, 842 - 846
14. Falorni, Massimo; Lardicci, Luciano; Uccello-Barretta, Gloria; Giacomelli, Giampaolo, Gazzetta Chimica Italiana, CODEN: GCITA9, 118(7), <1988>, 495 - 500
15. Suga, Takayuki; Hirata, Toshifumi; Hamada, Hiroki; Murakami, Satoru, Phytochemistry (Elsevier), CODEN: PYTCAS, 27(4), <1988>, 1041 - 1044
16. Suga, Takayuki; Hamada, Hiroki; Hirata, Toshifumi; Izumi, Shunsuke, Chemistry Letters, CODEN: CMLTAG, <1987>, 903 - 906
17. Hamada, Hiroki, Bulletin of the Chemical Society of Japan, CODEN: BCSJA8, 61, <1988>, 869 - 878
18. Komatsu; Kurata, Memoirs of the College of Science, Kyoto Imperial University, CODEN: MSKIAS, <A> 7, 152
19. Menon, Rani B.; Kumar, M. Anil; Ravindranathan, T., Tetrahedron Letters, CODEN: TELEAY, 28(44), <1987>, 5313 - 5314
20. Brieskorn, Carl Heinz; Ryu, Chung-Kyu, Archiv der Pharmazie (Weinheim, Germany), CODEN: ARPMAS, 318(3), <1985>, 261 - 270
21. Johnson, Carl R.; Zeller, James R., Tetrahedron, CODEN: TETRAB, 40(8), <1984>, 1225 - 1234
22. Duraisamy, M.; Walborsky, H. M., Journal of the American Chemical Society, CODEN: JACSAT, 105(10), <1983>, 3252 - 3264

Notes(s):

1. Only first 20 entries are displayed. Total number of entries = 39. Use "DIS F<prop>" for full format, e.g. FCPD instead of CPD.

Refractive Index:

Value (RI) (--)	Temp. (.T) (Cel)	Wavelen. (.W) (nm)	Ref.	Note
1.45	20	589	1	
1.4504	20	589	2, 3, 4	
1.4503	24	589	5	
1.4472	25	589	6	
1.4503	25	589	7	
1.4501	20	589	8	
1.4599	11	589	9	1
1.4481	25	589	10	

Reference(s):

1. Lochynski, Stanislaw; Kuldo, Joanna; Frackowiak, Bozena; Holband, Jolanta; Wojcik, Grazyna, Tetrahedron: Asymmetry, CODEN: TASYE3, 11(6), <2000>, 1295 - 1302
2. Zeitschel; Schmidt, Chemische Berichte, CODEN: CHBEAM, 59, <1926>, 2303
3. Huggett, Journal of the Society of Chemical Industry, London, CODEN: JSCIAN, 60, <1941>, 67, Quarterly Journal of Pharmacy and Pharmacology, CODEN: QJPPAL, 15, <1942>, 218
4. Odinokov, V. N.; Botsman, L. P.; Emel'yanova, G. A., Russian Chemical Bulletin, CODEN: RCBUEY, 47(10), <1998>, 2021 - 2022, Izvestiya Akademi Nauk, Seriya Khimicheskaya, CODEN: IASKEA(10), <1998>, 2077 - 2078
5. Odinokov, V. N.; Ishmuratov, G. Yu.; Yakovleva, M. P.; Muslukhov, R. R.; Safiullin, R. L.; et al., Doklady Chemistry, CODEN: DKCHAY, 326(4-6), <1992>, 231 - 235, Dokl. Akad. Nauk SSSR Ser. Khim., CODEN: DASKAJ, 326(5), <1992>, 842 - 846
6. Suga, Takayuki; Hirata, Toshifumi; Hamada, Hiroki; Murakami, Satoru, Phytochemistry (Elsevier), CODEN: PYTCAS, 27(4), <1988>, 1041 - 1044
7. Hamada, Hiroki, Bulletin of the Chemical Society of Japan, CODEN: BCSJA8, 61, <1988>, 869 - 878
8. Derdzinski,K.; Zabza,A., Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques, CODEN: BAPCAQ, 25, <1977>, 529 - 540
9. Grignard; Savard, Bulletin des Societes Chimiques Belges, CODEN: BSCBAG, 36, <1927>, 106, Chem. Zentralbl., CODEN: CHZEA6, 98(I), <1927>, 2998
10. Hiraidzumi, Chikashige-Festschr. <Kyoto 1930> S. 85, 86

Notes(s):

1. Refractive index:Enolform des Menthons, p-Menthen-(3)-ol-(3).

Liquid Density:

Value (DEN) (g/cm**3)	Temp. (.T) (Cel)	Ref. Temp. (.RT) (Cel)	Ref.	Note
	25		1	
0.8954	20	4	2	
	20		3	
0.8869	30	4	4	
0.893	11	4	5	1
0.8964	15	4	6	
0.8885	25	4	7	
0.8903	25	4	8	

Reference(s):

1. Suga, Takayuki; Hirata, Toshifumi; Hamada, Hiroki; Murakami, Satoru Phytochemistry (Elsevier), CODEN: PYTCAS, 27(4), <1988>, 1041 - 1044
2. Khunt,V.N. et al., Journal of the Indian Chemical Society, CODEN: JICSAH, 56, <1979>, 436 - 437
3. Huggett, Journal of the Society of Chemical Industry, London, CODEN: JSCIAN, 60, <1941>, 67, Quarterly Journal of Pharmacy and Pharmacology, CODEN: QJPPAL, 15, <1942>, 218
4. Gillespie; Macbeth; Mills, Journal of the Chemical Society, CODEN: JCSOA9, <1940>, 280
5. Grignard; Savard, Bulletin des Societes Chimiques Belges, CODEN: BSCBAG, 36, <1927>, 106, Chem. Zentralbl., CODEN: CHZEA6, 98(I), <1927>, 2998
6. Zeitschel; Schmidt, Chemische Berichte, CODEN: CHBEAM, 59, <1926>, 2303
7. Hiraidzumi, Chikashige-Festschr. <Kyoto 1930> S. 85, 86
8. Komatsu; Kurata, Memoirs of the College of Science, Kyoto Imperial University, CODEN: MSKIAS, <A> 7, 152

Notes(s):

1. Enolform des Menthons, p-Menthen-(3)-ol-(3).

Solubility (MCS):

Value (SLB) (g/L)	Saturation (.SAT)	Temp. (.T) (Cel)	Solvent (.SOL)	Ref.	Note
10.9826	in pure solvent	25	H2O, various solvent(s)	1	1
1.4191	in pure solvent	25	H2O, various solvent(s)	1	1
1.3574	in pure solvent	25	H2O, various solvent(s)	1	1
0.4319	in pure solvent	25	H2O, various solvent(s)	1	1
0.3085	in pure solvent	25	H2O	1	
	in pure solvent			2	2

Reference(s):
1. Ajisaka, Noriko; Hara, Koji; Mikuni, Katsuhiko; Hara, Kozo; Hashimoto, Hitoshi, Bioscience, Biotechnology, and Biochemistry, CODEN: BBBIEJ, 64(4), <2000>, 731 - 734
2. Ruelle, Paul; Kesselring, Ulrich W., Journal of Pharmaceutical Sciences, CODEN: JPMSAE, 87(8), <1998>, 998 - 1014

Notes(s):
1. in the presence of organic compounds
2. equation

Pharmacological Data:

PHARM

Effect (.E):	cell permeability; enhancement of
Species or Test-System (.SP):	colon HTB-37 Caco-2 cells of human
Kind of Dosing (.KD):	title comp. dissolved in Dulbecco's Modified Eagles Medium (DMEM) and used at concentrations of 1, 0.1 and 0.01percent w/v
Method, Remarks (.MR):	cells transferred into a 24-well BD Falcon plate and 1 ml of DMEM applied to basolateral compartment; title comp. applied to apical compartment; transepithelial electrical resistance measured; enhancement potential measured
Further Details (.FD):	positive control: Triton X-100; enhancement potential were on a scale of 0 to 1, with 1 representing maximum enhancement compared to positive control
Results (.RE):	enhancement potential of title comp. at 1, 0.1 and 0.01percent were 0.89, 0.28 and 0.17, resp.; table

Reference(s):
1. Whitehead, Kathryn; Mitragotri, Samir, Pharmaceutical Research, CODEN: PHREEB, 25(6), <2008>, 1412 - 1419

PHARM

Effect (.E):	cytotoxicity
Species or Test-System (.SP):	colon HTB-37 Caco-2 cells of human
Kind of Dosing (.KD):	title comp. dissolved in Dulbecco's Modified Eagles Medium; 100 .my.l used at concentrations of 1, 0.1 and 0.01percent w/v
Method, Remarks (.MR):	cells seeded onto 96-well plate; title comp. applied for 30 min; MTT assay performed; toxicity potential of title comp. calculated as fraction of nonviable cells following title comp. treatment compared to negative control
Further Details (.FD):	negative control: Dulbecco's Modified Eagles Medium; toxicity potential values ranged from 0 to 1, with 0 indicating no mitochondrial toxicity, and 1 representing maximum toxicity
Results (.RE):	toxicity potential of title comp. at 1, 0.1 and 0.01percent were 0.37, 0.01 and 0.02, resp.; table

Reference(s):
1. Whitehead, Kathryn; Mitragotri, Samir, Pharmaceutical Research, CODEN: PHREEB, 25(6), <2008>, 1412 - 1419

PHARM

Effect (.E):	cytotoxicity
Species or Test-System (.SP):	colon HTB-37 Caco-2 cells of human
Kind of Dosing (.KD):	title comp. dissolved in Dulbecco's Modified Eagles Medium; 100 .my.l used at concentrations of 1, 0.1 and 0.01percent w/v

```
      Method, Remarks (.MR):              cells seeded onto 96-well plate; title
                                          comp. applied for 30 min; lactate
                                          dehydrogenase (LDH) reagent added;
                                          incubated; absorbance measured at 490 nm;
                                          LDH potential calculated as fraction of
                                          maximal LDH release
      Further Details (.FD):              positive control: 1percent Triton-X-100;
                                          LDH potential values ranged from 0 to 1,
                                          with 0 indicating no LDH release, and 1
                                          representing maximum LDH release
      Results (.RE):                      LDH potential of title comp. at 1, 0.1 and
                                          0.01percent were 0.42, 0.11 and 0.09,
                                          resp.; table
      Reference(s):
      1.  Whitehead, Kathryn; Mitragotri, Samir, Pharmaceutical Research, CODEN:
          PHREEB, 25(6), <2008>, 1412 - 1419
PHARM
      Effect (.E):                        cell permeability; enhancement of
      Species or Test-System (.SP):       colon Caco-2 HTB-37 cells of human
      Kind of Dosing (.KD):               title comp. dissolved in Dulbecco's
                                          Modified Eagles Medium (DMEM) and used at
                                          concentrations of 1, 0.1 and 0.01percent
                                          w/v
      Method, Remarks (.MR):              cells transferred into a 24-well BD Falcon
                                          plate and 1 ml of DMEM applied to
                                          basolateral compartment; title comp.
                                          applied to apical compartment;
                                          transepithelial electrical resistance
                                          measured at 10 min; enhancement potential
                                          measured
      Further Details (.FD):              positive control: Triton X-100;
                                          enhancement potential were on a scale of 0
                                          to 1, with 1 representing maximum
                                          enhancement compared to positive control
      Results (.RE):                      enhancement potential of title comp. at 1,
                                          0.1 and 0.01percent were 0.89, 0.28 and
                                          0.17, resp.; table
      Reference(s):
      1.  Whitehead, Kathryn; Karr, Natalie; Mitragotri, Samir, Pharmaceutical
          Research, CODEN: PHREEB, 25(8), <2008>, 1782 - 1788
PHARM
      Effect (.E):                        cytotoxicity
      Species or Test-System (.SP):       colon Caco-2 HTB-37 cells of human
      Kind of Dosing (.KD):               title comp. dissolved in Dulbecco's
                                          Modified Eagles Medium; 100 .my.l used at
                                          concentrations of 1, 0.1 and 0.01percent
                                          w/v
      Method, Remarks (.MR):              cells seeded onto 96-well plate; title
                                          comp. applied for 30 min; MTT assay
                                          performed; toxicity potential of title
                                          comp. calculated as fraction of nonviable
                                          cells following title comp. treatment
                                          compared to negative control
      Further Details (.FD):              negative control: Dulbecco's Modified
                                          Eagles Medium; toxicity potential values
                                          ranged from 0 to 1, with 0 indicating no
                                          mitochondrial toxicity, and 1 representing
                                          maximum toxicity
      Results (.RE):                      toxicity potential of title comp. at 1,
                                          0.1 and 0.01percent were 0.37, 0.01 and
                                          0.02, resp.; table
      Reference(s):
      1.  Whitehead, Kathryn; Karr, Natalie; Mitragotri, Samir, Pharmaceutical
          Research, CODEN: PHREEB, 25(8), <2008>, 1782 - 1788
PHARM
      Effect (.E):                        agonist
      Species or Test-System (.SP):       HEK293 cell expressing murine TRPV3 ion
                                          channel
      Concentration (.C):                 2 mmol/l
      Kind of Dosing (.KD):               dissolved in assay buffer
      Method, Remarks (.MR):              whole-cell mode of the patch-clamp
                                          technique; recordings were carried out at
                                          32 deg C; cell was held at -40 mV and
                                          transiently perfused with title comp. for
                                          10 s; before each recording, cell
                                          sensitized with 10-15 pulses of 2-APB (300
                                          .my.M)
      Further Details (.FD):              HEK293: human embryonic kidney 293; TRP:
                                          transient receptor potential; 2-APB:
                                          2-aminoethoxydiphenyl borate; result
```

```
                                    expressed as percentage of current evoked
                                    by camphor (2 mM)
     Results (.RE):                 20percent activation
     Reference(s):
     1.  Vogt-Eisele, A. K.; Weber, K.; Sherkheli, M. A.; Vielhaber, G.; Panten,
         J.; Gisselmann, G.; Hatt, H., British Journal of Pharmacology, CODEN:
         BJPCBM, 151(4), <2007>, 530 - 540
PHARM
     Effect (.E):                   agonist
     Species or Test-System (.SP):  Hek293 cell expressing murine TRPM8 ion
                                    channel
     Concentration (.C):            2 mmol/l
     Kind of Dosing (.KD):          dissolved in assay buffer
     Method, Remarks (.MR):         whole-cell mode of the patch-clamp
                                    technique; recordings were carried out at
                                    22 -25 deg C; cell was held at -40 mV and
                                    transiently perfused with title comp. for
                                    5 s
     Further Details (.FD):         HEK293: human embryonic kidney 293; TRP:
                                    transient receptor potential; result
                                    expressed as percentage of current evoked
                                    by (-)-menthol (2 mM)
     Results (.RE):                 title comp. resulted in ca. <10percent
                                    activation; fig.
     Reference(s):
     1.  Vogt-Eisele, A. K.; Weber, K.; Sherkheli, M. A.; Vielhaber, G.; Panten,
         J.; Gisselmann, G.; Hatt, H., British Journal of Pharmacology, CODEN:
         BJPCBM, 151(4), <2007>, 530 - 540
PHARM
     Effect (.E):                   biotransformation
     Species or Test-System (.SP):  liver microsomes of human
     Kind of Dosing (.KD):          200 .my.M of title comp. diluted in final
                                    volume 0.50 ml of 100 nM aq. potassium
                                    phosphate buffer
     Method, Remarks (.MR):         incubation of title comp. with microsomes
                                    in presence of NADPH-generating system;
                                    GC-MS analysis of reaction mixture
     Further Details (.FD):         reaction mixture without microsomes used
                                    as blank experiment
     Metabolite AN (.AN):           2037488, 11116873
     Metabolite (.META):            (1S,2S,5R)-2-isopropyl-5-methylcyclohexano
                                    l, 7-hydroxymenthone
     Reference(s):
     1.  Miyazawa, Mitsuo; Nakanishi, Kyousuke, Bioscience, Biotechnology, and
         Biochemistry, CODEN: BBBIEJ, 70(5), <2006>, 1259 - 1261
PHARM
     Effect (.E):                   efflux; inhibition of
     Species or Test-System (.SP):  porcine kidney LLC-PK1 cells expressing
                                    human MDR1 cDNA
     Concentration (.C):            1 mmol/l
     Kind of Dosing (.KD):          vehicle: Hanks' balanced salt solution
                                    with 1percent dimethyl sulfoxide
     Method, Remarks (.MR):         cell monolayers incubated with 30 nM
                                    <3H>digoxin in presence of title comp. for
                                    1 h; P-glycoprotein (P-gp)-mediated efflux
                                    determined by measuring cell-to-medium
                                    ratio of <3H>digoxin
     Further Details (.FD):         reference comp.: SDZ-PSC833 and verapamil;
                                    MDR1 gene: encodes P-glycoprotein
     Note(s) (.COM):                No effect
     Reference(s):
     1.  Yoshida, Naoko; Koizumi, Mariya; Adachi, Isao; Kawakami, Junichi, Food
         and Chemical Toxicology, CODEN: FCTOD7, 44(12), <2006>, 2033 - 2039
PHARM
     Effect (.E):                   cytotoxicity
     Species or Test-System (.SP):  porcine kidney LLC-PK1 cells expressing
                                    human MDR1 cDNA
     Concentration (.C):            1 mmol/l
     Method, Remarks (.MR):         cells incubated with title comp. for 1 h;
                                    cells viability assessed by measuring
                                    leakage of lactate dehydrogenase (LDH)
                                    into medium using commercial test
     Further Details (.FD):         MDR1 gene: encodes P-glycoprotein
     Note(s) (.COM):                No effect
     Reference(s):
     1.  Yoshida, Naoko; Koizumi, Mariya; Adachi, Isao; Kawakami, Junichi, Food
         and Chemical Toxicology, CODEN: FCTOD7, 44(12), <2006>, 2033 - 2039
```

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PHARM
     Effect (.E):                        cytotoxicity
     Species or Test-System (.SP):       human colorectal carcinoma Caco-2 cells
     Concentration (.C):                 1 mmol/l
     Method, Remarks (.MR):              cells incubated with title comp. for 1 h;
                                         cells viability assessed by measuring
                                         leakage of lactate dehydrogenase (LDH)
                                         into medium using commercial test
     Note(s) (.COM):                     No effect
     Reference(s):
     1.  Yoshida, Naoko; Koizumi, Mariya; Adachi, Isao; Kawakami, Junichi, Food
         and Chemical Toxicology, CODEN: FCTOD7, 44(12), <2006>, 2033 - 2039
PHARM
     Effect (.E):                        transdermal permeation enhancer
     Species or Test-System (.SP):       abdominal human skin
     Sex (.S):                           female
     Kind of Dosing (.KD):               title comp. solution in propylene glycol
                                         20:80 (w/w)
     Method, Remarks (.MR):              skin pieces mounted in diffusion cells at
                                         32 deg C and pH 7.4; title comp. solution
                                         added into donor compartment, 6 h later
                                         aspirated; skin surface rinsed; alprazolam
                                         added into donor compartment; receptor
                                         solution samples analyzed for 24 h by
                                         HPLC-UV
     Further Details (.FD):              cell with no title comp. applied used to
                                         obtain baseline permeation profile of
                                         alprazolam
     Results (.RE):                      title comp. ca. 10 times increased
                                         permeation parameters of alprazolam
                                         figure)
     Reference(s):
     1.  Boix, A.; Peraire, C.; Obach, R.; Domenech, J., Pharmaceutical
         Research, CODEN: PHREEB, 22(1), <2005>, 94 - 102
PHARM
     Effect (.E):                        anaesthetic
     Species or Test-System (.SP):       New Zealand albino rabbit
     Route of Application (.RA):         conjunctival
     Concentration (.C):                 3 - 1000 mg/l
     Kind of Dosing (.KD):               title comp. in DMSO-water administered
                                         into the conjunctival sac
     Method, Remarks (.MR):              conjunctival reflex test according to
                                         Donatelli and Buffoni; external side of
                                         eye stimulated with a cat whisker to
                                         induce conjunctival reflex, closure of
                                         palpebrals
     Further Details (.FD):              rabbit wt 2.5-3.0 kg
     Results (.RE):                      no local anaesthetic effect; graphical
                                         representations
     Reference(s):
     1.  Galeotti, Nicoletta; Ghelardini, Carla; Mannelli, Lorenzo Di Cesare;
         Mazzanti, Gabriela; Baghiroli, Laura; Bartolini, Alessandro, Planta
         Medica, CODEN: PLMEAA, 67(2), <2001>, 174 - 176
PHARM
     Effect (.E):                        anaesthetic
     Species or Test-System (.SP):       Wistar rat phrenic nerve-hemidiaphragm
     Sex (.S):                           male
     Concentration (.C):                 0.0001 - 1 mg/l
     Method, Remarks (.MR):              method according to Buelbring and Wessler
                                         and Kilbinger;
     Further Details (.FD):              rat wt 150-200 g
     Results (.RE):                      no reduction of the electrically evoked
                                         contractions of phrenic hemidiaphragm;
                                         graphical representation
     Reference(s):
     1.  Galeotti, Nicoletta; Ghelardini, Carla; Mannelli, Lorenzo Di Cesare;
         Mazzanti, Gabriela; Baghiroli, Laura; Bartolini, Alessandro, Planta
         Medica, CODEN: PLMEAA, 67(2), <2001>, 174 - 176
PHARM
     Effect (.E):                        antithrombotic
     Species or Test-System (.SP):       Japanese white rabbit blood
     Sex (.S):                           male
     Method, Remarks (.MR):              PRP (platelet-rich plasma) and PPP
                                         (platelet poor plasma) separated by
                                         centrifugation; platelet aggregation in
                                         PRP initiated by Na-arachidonate, detd.
                                         turbidimetrically
     Results (.RE):                      inhibited platelet aggregation by 17
                                         percent
```

```
      Reference(s):
      1.  Enomoto, Shigeki; Asano, Ryoya; Iwahori, Yoshihiro; Narui, Takao;
          Okada, Yoshihito; Singab, Abdel Nasser B.; Okuyama, Toru, Biological &
          Pharmaceutical Bulletin, CODEN: BPBLEO, 24(3), <2001>, 307 - 310
PHARM
      Effect (.E):                          antimutagenic
      Species or Test-System (.SP):         Salmonella typhimurium TA1535/pSK1002
      Concentration (.C):                   0.01 - 1 mmol/l
      Method, Remarks (.MR):                in vitro; suppression of
                                            furylfuramide-induced SOS response
                                            examined using umu test
      Type (.TYP):                          ID50
      Value of Type (.V):                   0.79 mmol/l
      Results (.RE):                        at 1.0 .my.mol/ml title comp. suppressed
                                            furylfuramide-induced SOS response by 61.1
                                            percent (conc.-response curve)
      Reference(s):
      1.  Miyazawa, Mitsuo; Okuno, Yoshiharu; Nakamura, Sei-ichi; Kosaka,
          Hiroshi, Journal of Agricultural and Food Chemistry, CODEN: JAFCAU,
          48(11), <2000>, 5440 - 5443
PHARM
      Note(s) (.COM):                       predicted nasal pungency threshold (NPT)
                                            89 ppm
      Reference(s):
      1.  Abraham, Michael H.; Kumarsingh, Rachel; Cometto-Muniz, J. Enrique;
          Cain, William S.; Roses, Marti; et al., Journal of the Chemical
          Society, Perkin Transactions 2:  Physical Organic Chemistry
          (1972-1999), CODEN: JCPKBH(11), <1998>, 2405 - 2412
PHARM
      Note(s) (.COM):                       inhibition of acetylcholinesterase
                                            activity: IC50 = 1.42 mM
      Reference(s):
      1.  Miyazawa, Mitsuo; Watanabe, Hitomi; Kameoka, Hiromu, Journal of
          Agricultural and Food Chemistry, CODEN: JAFCAU, 45(3), <1997>, 677 -
          679
PHARM
      Note(s) (.COM):                       in vitro destruction of rat liver
                                            microsomal cytochrome P-450 (40.92percent
                                            loss) but not heme (0percent loss) by the
                                            drug (10 mM) at 37 deg C for 15 min
      Reference(s):
      1.  Moorthy, B; Madyastha, P; Madyastha, K M, Indian Journal of Chemistry,
          Section B:  Organic Chemistry Including Medicinal Chemistry, CODEN:
          IJSBDB, 30(2), <1991>, 138 - 146
PHARM
      Note(s) (.COM):                       in vitro destruction of rat liver
                                            microsomal cytochrome P-450 (41.4percent
                                            loss) but not heme (0percent loss) by the
                                            drug (10 mM) in the presence of 1 mM NADPH
                                            at 37 deg C for 15 min
      Reference(s):
      1.  Moorthy, B; Madyastha, P; Madyastha, K M, Indian Journal of Chemistry,
          Section B:  Organic Chemistry Including Medicinal Chemistry, CODEN:
          IJSBDB, 30(2), <1991>, 138 - 146
```

Example 2: REACH relevant data for an inorganic substance (S <MF>, D REACH)

```
Accession Number (AN):                  16474443
      Chemical Name (CN):               anatase O2Ti, titanium(IV) oxide,
       titanium
                                        dioxide, anatase titania, titaniumdioxide,
                                        titanium oxide, titanium
      Lin. Struct. Formula (LSF):       TiO2.0
      Molec. Formula (MF):              O2 Ti
      Formula Weight (FW):              79.8788
      Compound Type (CTYPE):            Mineral, Solid solution, Glass or Ceramic
                                        material
      InChi Key: (INCHI):               QWWIMOOFEDJKFN-UHFFFAOYSA-N
      Alternate InChi Key: (AINCHI):    QWWIMOOFEDJKFN-UHFFFAOYAE
      Markush Ref. Count (MARKREF):     0
      Entry Date (DED):                 2008/10/13
      Update Date (DUPD):               2011/03/21

      No structure diagram available for this Document

    Field Availability:

      Code      Name                                Occurrence
      ========================================================
      AN        Accession Number                             1
      CN        Chemical Name                                7
      LSF       Linearized Structure Formula                 1
      MF        Molecular Formula                            1
      FW        Formula Weight                               1
      INCHI     InChi Key                                    1
      AINCHI    Alternate InChi Key                          1
      CTYPE     Compound Type                                3
      MARKREF   Markush Reference Count                      1
      DED       Entry Date                                   1
      DUPD      Update Date                                  1
      ADSM      Adsorption (MCS)                            28
      ASSM      Association (MCS)                            1
      CDEN      Density (Crystal)                           27
      CNF       Conformation                                 1
      CP        Heat Capacity Cp                           103
      CPD       Crystal Property Description                22
      CRYPH     Crystal Phase                               22
      CSG       Crystal Space Group                        164
      CSYS      Crystal System                               4
      CTP       Crystal Transition Point                     1
      DFM       Molecular Deformation                        1
      DIC       Dielectric Constant                          4
      ELCH      Electrochemistry Data                       16
      ELE       Electrical Data (MCS)                        5
      ESR       ESR Data                                    54
      FINFO     Further Information                        593
      FLU       Fluorescence                                 1
      GEO       Interatomic Distanc and Angle                3
      IR        Infrared Spectrum                          138
      LUM       Luminescence                                 2
      MAG       Magnetic Data                                4
      MEC       Mechanical Property                          6
      MSUS      Magnetic Susceptibility                      4
      NMR       Nuclear Magnetic Resonance                   8
      OPT       Optics                                       2
      OSM       Other Spectroscopic Methods                  4
      PHARM     Pharmacological Data                         1
      POT       Electrochemical Characteristics             20
      QCC       Quantum Chemical Calculations               42
      RAS       Raman Spectrum                               1
      RI        Refractive Index                            17
      SLB       Solubility (MCS)                             2
      TEC       Thermal Expansion                           46
      TRAM      Transport Phenomena (MCS)                    5
      USC       Use of Compound                             11
      UVS       UV and Visible Spectrum                    171
```

This substance also occurs in Reaction Documents:

Code	Name	Occurrence
RX	Reaction Documents	1294
RX.RAN	Reactant AN	941
RX.PAN	Product AN	353

Refractive Index:

Value (RI) (--)	Temp. (.T) (Cel)	Wavelen. (.W) (nm)	Ref.	Note
2.5			1	
1.55			2	1
2.08			2	
2.16		1900	3	2
2.29		633	3	3
1.9			4	4
2.3			4	5
2.4447	25	690.75	5, 6	6
2.488	25	589.3	5, 6	6
2.488 - 2.4886		589.3	7, 6	6
2.5097	25	690.75	5, 6	7
2.5161	25	456.07	5, 6	6
2.5612	25	589.3	5, 6	7
2.5612 - 2.5618		589.3	7, 6	7
2.5948	25	456.07	5, 6	7
2.6576	25	435.83	5, 6	6
2.7688	25	435.83	5, 6	7

Reference(s):
1. Waterhouse, Geoffrey I. N.; Waterland, Mark R., Polyhedron, CODEN: PLYHDE, 26, <2007>, 356 - 368
2. Arimitsu, Naoki; Nakajima, Akira; Saito, Keisuke; Kameshima, Yoshikazu; Okada, Kiyoshi, Chemistry Letters, CODEN: CMLTAG, 36, <2007>, 106 - 107
3. Hashimoto, Tadanori; Yoko, Toshinobu; Sakka, Sumio, Bulletin of the Chemical Society of Japan, CODEN: BCSJA8, 67, <1994>, 653 - 660
4. Khodos, M. Ya.; Krivosheev, N. V.; Teterin, G. A.; Alekseev, O. G.; Zuravlev, Yu. F., Inorganic Materials (Transl. of Neorg. Mater.), CODEN: INOMAF, 26, <1990>, 484 - 488, Izvestiya Akademii Nauk SSSR, Neorganicheskie Materialy, CODEN: IVNMAW, 26, <1990>, 573 - 577
5. , Ti: MVol., 5.3.3, page 226 - 255
6. Schroeder, A., Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie, CODEN: ZKKKAJ, 67, <1928>, 485 - 542
7. , Ti: MVol., 1.1, page 70 - 75

Notes(s):
1. as-coated
2. n.vpi.
3. n3.vpi.
4. amorphous
5. crystalline
6. nε
7. nω

Solubility (MCS):

Value (SLB) (g/L)	Ref.	Note
	1	1
	2, 3	2

Reference(s):
1. Chaliyan, K. N., Radiokhimiya, CODEN: SVRDAX, 26, <1984>, 370 - 372, Radiokhimiya, CODEN: RADKAU, 26, <1984>, 390 - 392
2. , Cl: MVol., 167, page 439 - 441
3. Treadwell, F. P., Lehrbuch der analytischen Chemie, 1. Bd., 12. Aufl., Leipzig-Wien 1922, S. 439

Notes(s):
1. insol. in water
2. insol. in aqua regia;

Heat Capacity (CP):

Value (CP) (J/mol*K)	Temp. (.T) (Cel)	Ref.	Note
		1, 2, 3, 4	1
16.62	-192.986	5	
17.724	-189.507	5	
19.26	-186.184	5	
20.782	-182.986	5	
21.761	-179.858	5	
22.84	-176.902	5	
24.149	-173.149	5	
25.631	-169.897	5	
26.568	-166.58	5	
28.062	-163.338	5	
29.504	-158.989	5	
30.578	-155.45	5	
31.592	-152.857	5	
32.26	-150.428	5	
32.873	-148.136	5	
33.812	-145.775	5	
34.982	-141.649	5	
36.546	-136.188	5	
38.444	-130.736	5	2

Reference(s):

1. Ding, Xing-Zhao; Liu, Xiang-Huai, Physica Status Solidi A: Applied Research, CODEN: PSSABA, 158, <1996>, 433 - 440
2. Dames, C.; Poudel, B.; Wang, W. Z.; Huang, J. Y.; Ren, Z. F.; et al., Applied Physics Letters, CODEN: APPLAB, 1 - 3, Applied Physics Letters, CODEN: APPLAB, 87, <2005>
3. , Ti: MVol., 5.3.3, page 226 - 255
4. Shomate, C. H., Journal of the American Chemical Society, CODEN: JACSAT, 69, <1947>, 218 - 219
5. Wu, Xin-Ming; Wang, Lan; Tan, Zhi-Cheng; Li, Guang-Hai; Qu, Song-Sheng, Journal of Solid State Chemistry, CODEN: JSSCBI, 156, <2001>, 220 - 224

Notes(s):

1. |Cp diagram
2. Only first 20 entries are displayed. Total number of entries = 103. Use "DIS F<prop>" for full format, e.g. FCPD instead of CPD.

Pharmacological Data:

PHARM

Note(s) (.COM): physiological behaviour discussed

Reference(s):

1. Daoud, Walid A.; Xin, John H.; Zhang, Yi-He, Surface Science, CODEN: SUSCAS, 599, <2005>, 69 - 75
2. Cai, Ruxiong; Hashimoto, Kazuhito; Itoh, Kiminori; Kubota, Yoshinobu; Fujishima, Akira, Bulletin of the Chemical Society of Japan, CODEN: BCSJA8, 64, <1991>, 1268 -