

# 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:

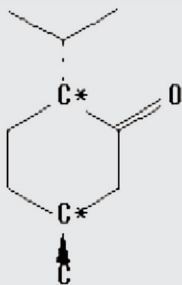
- Melting Point (MP)
- Sublimation Point (SP)
- Boiling Point (BP)
- Vapor Pressure (VP)
- Optical Rotatory Power (ORP)
- Refractive Index (RI)
- Mutarotation (MUT)
- Liquid Density (DEN)
- Dissociation Exponent (DE)
- Solubility (SLB)
- Heat Capacity (CP)
- Heat Capacity (CV)
- Enthalpy of Formation (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):

- 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
- Fischer, Bulletin des Societes Chimiques Belges, CODEN: BSCBAG, 49, <1940>, 129,133
- 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):

- Jain, Suman L.; Sharma, Vishal B.; Sain, Bir, Tetrahedron, CODEN: TETRAB, 62(29), <2006>, 6841 - 6847
- 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
- Mohajerani, Bagher; Heravi, Majid M.; Ajami, Dariush, Monatshefte fuer Chemie, CODEN: MOCMB7, 132(7), <2001>, 871 - 874
- Lochynski, Stanislaw; Kuldo, Joanna; Frackowiak, Bozena; Holband, Jolanta; Wojcik, Grazyna, Tetrahedron: Asymmetry, CODEN: TASYE3, 11(6), <2000>, 1295 - 1302
- Chen, Fener; Liu, Anchang; Yan, Qiongjiao; Liu, Mingxing; Zhang, Daoming; Shao, Lanying, Synthetic Communications, CODEN: SYNCAV, 29(6), <1999>, 1049 - 1056
- 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 Akademii 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):**

- Lochynski, Stanislaw; Kuldo, Joanna; Frackowiak, Bozena; Holband, Jolanta; Wojcik, Grazyna, *Tetrahedron: Asymmetry*, CODEN: TASYE3, 11(6), <2000>, 1295 - 1302
- Zeitschel; Schmidt, *Chemische Berichte*, CODEN: CHBEAM, 59, <1926>, 2303
- 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
- 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
- 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
- Suga, Takayuki; Hirata, Toshifumi; Hamada, Hiroki; Murakami, Satoru, *Phytochemistry (Elsevier)*, CODEN: PYTCAS, 27(4), <1988>, 1041 - 1044
- Hamada, Hiroki, *Bulletin of the Chemical Society of Japan*, CODEN: BCSJA8, 61, <1988>, 869 - 878
- Derdzinski, K.; Zabza, A., *Bulletin de l'Academie Polonaise des Sciences, Serie des Sciences Chimiques*, CODEN: BAPCAQ, 25, <1977>, 529 - 540
- Grignard; Savard, *Bulletin des Societes Chimiques Belges*, CODEN: BSCBAG, 36, <1927>, 106, *Chem. Zentralbl.*, CODEN: CHZEA6, 98(I), <1927>, 2998
- Hiraidzumi, *Chikashige-Festschr. <Kyoto 1930> S. 85, 86*

**Notes(s):**

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

**Liquid Density:**

Value (DEN) (g/cm <sup>3</sup> )	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):**

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

**Notes(s):**

- 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):

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

## Notes(s):

- in the presence of organic compounds
- 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 . $\mu$ 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 . $\mu$ 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)  
 20percent activation

Results (.RE):  
 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 1, 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

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):                   QWWIMOOFEJJKFN-UHFFFAOYSA-N
Alternate InChi Key: (AINCHI):        QWWIMOOFEJJKFN-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):

- Waterhouse, Geoffrey I. N.; Waterland, Mark R., Polyhedron, CODEN: PLYHDE, 26, <2007>, 356 - 368
- Arimitsu, Naoki; Nakajima, Akira; Saito, Keisuke; Kameshima, Yoshikazu; Okada, Kiyoshi, Chemistry Letters, CODEN: CMLTAG, 36, <2007>, 106 - 107
- Hashimoto, Tadanori; Yoko, Toshinobu; Sakka, Sumio, Bulletin of the Chemical Society of Japan, CODEN: BCSJA8, 67, <1994>, 653 - 660
- 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
- , Ti: MVol., 5.3.3, page 226 - 255
- Schroeder, A., Zeitschrift fuer Kristallographie, Kristallgeometrie, Kristallphysik, Kristallchemie, CODEN: ZKKKAJ, 67, <1928>, 485 - 542
- , Ti: MVol., 1.1, page 70 - 75

#### Notes(s):

- as-coated
- n.vpi.
- n3.vpi.
- amorphous
- crystalline
- nE
- nW

#### Solubility (MCS):

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

#### Reference(s):

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

#### Notes(s):

- insol. in water
- 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):

- Ding, Xing-Zhao; Liu, Xiang-Huai, *Physica Status Solidi A: Applied Research*, CODEN: PSSABA, 158, <1996>, 433 - 440
- 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>
- , Ti: MVol., 5.3.3, page 226 - 255
- Shomate, C. H., *Journal of the American Chemical Society*, CODEN: JACSAT, 69, <1947>, 218 - 219
- 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):

- |Cp diagram
- 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):

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