

Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1S-endo)-

Other names:

Borneol, (1S,2R,4S)-(-)-
(-)-Borneol
L-Borneol
Linderol
Ngai camphor
((1S)-endo)-(-)-Borneol
l-2-Bornanol
1-Bornyl alcohol
l-2-Camphanol
(-)-(1S,4S)-Borneol
(1S-endo)1,7,7-Trimethyl-bicyclo[2.2.1]heptan-2-ol
Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1S,2R,4S)-
(1S,2R,4S)-1,7,7-Trimethylbicyclo[2.2.1]heptan-2-ol
(1S)-endo-Borneol
Borneol
endo(-)-Borneol
endo-(1S)-(-)-Borneol

Inchi: InChI=1S/C10H18O/c1-9(2)7-4-5-10(9,3)8(11)6-7/h7-8,11H,4-6H2,1-3H3/t7?,8-,10?/m1/s

InchiKey: DTGKSKDOIYIVQL-CCNFQMFXSA-N

Formula: C10H18O

SMILES: CC1(C)C2CCC1(C)C(O)C2

Mol. weight [g/mol]: 154.25

CAS: 464-45-9

Physical Properties

Property code	Value	Unit	Source
gf	-20.50	kJ/mol	Joback Method
hf	-272.72	kJ/mol	Joback Method
hfus	9.46	kJ/mol	Joback Method
hvap	51.61	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.194		Crippen Method
mcvol	135.910	ml/mol	McGowan Method
pc	3166.83	kPa	Joback Method
rinpol	1124.00		NIST Webbook
rinpol	1152.00		NIST Webbook
rinpol	1173.00		NIST Webbook

rmpol	1160.00		NIST Webbook
rmpol	1166.00		NIST Webbook
rmpol	1160.00		NIST Webbook
rmpol	1124.00		NIST Webbook
ripol	1675.00		NIST Webbook
ripol	1675.00		NIST Webbook
tb	486.55 ± 0.50	K	NIST Webbook
tb	483.20	K	NIST Webbook
tc	730.21	K	Joback Method
tf	334.96	K	Joback Method
vc	0.514	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.30	J/mol×K	529.27	Joback Method
cpg	370.25	J/mol×K	562.76	Joback Method
cpg	385.05	J/mol×K	596.25	Joback Method
cpg	398.92	J/mol×K	629.74	Joback Method
cpg	412.02	J/mol×K	663.23	Joback Method
cpg	424.55	J/mol×K	696.72	Joback Method
cpg	436.70	J/mol×K	730.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C464459&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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