epi-Borneol

Other names: 1,7,7-trimethyl-exo-bicyclo[2.2.1]heptan-2-ol
bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, (1R,2R,4R)-rel-
exo-isoborneol
exo-isobornyl alcohol
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-MRTMQBJTSA-N
Formula: C10H18O
SMILES: CC1(C)C2CCC1(C)C(O)C2
Mol. weight [g/mol]: 154.25

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	1164.00		NIST Webbook
tb	529.27	K	Joback Method
tc	730.21	K	Joback Method
tf	334.96	K	Joback Method
tt	482.70	K	Determination and Correlation of Solubility of Borneol, Camphor, and Isoborneol in Different Solvents
vc	0.514	m3/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

Determination and Correlation of Solubility of Borneol, Camphor, and Isoborneol in Different Solvents:	https://www.doi.org/10.1021/acs.jced.9b00045
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=R324862&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume