(S)-camphor

Other names:	(-)-2-bornanone (-)-alcanfor (-)-camphor (1S)-(-)-camphor (1S)-1,7,7-trimethylbicyclo[2.2.1]heptan-2-one bicyclo[2.2.1]heptan-2-one, 1,7,7-trimethyl-, (1S)- camphor, (1S,4S)-(-)- l-camphor
Inchi:	InChI=1S/C10H16O/c1-9(2)7-4-5-10(9,3)8(11)6-7/h7H,4-6H2,1-3H3/t7-,10+/m0/s1
InchiKey:	DSSYKIVIOFKYAU-OIBJUYFYSA-N
Formula:	C10H16O
SMILES:	CC12CCC(CC1=O)C2(C)C
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	1.44	kJ/mol	Joback Method
hf	-237.85	kJ/mol	Joback Method
hfus	3.81	kJ/mol	Joback Method
hvap	39.49	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	2.402		Crippen Method
mcvol	131.610	ml/mol	McGowan Method
pc	3082.99	kPa	Joback Method
rinpol	1142.00		NIST Webbook
rinpol	1142.00		NIST Webbook
ripol	1509.00		NIST Webbook
ripol	1509.00		NIST Webbook
tb	509.58	K	Joback Method
tc	742.46	K	Joback Method
tf	346.60	K	Joback Method
tt	453.90	K	Dielectric and thermodynamic study of camphor and borneol enantiomers and their binary systems
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.29	J/mol×K	509.58	Joback Method
cpg	342.61	J/mol×K	548.39	Joback Method
cpg	359.48	J/mol×K	587.21	Joback Method
cpg	375.18	J/mol×K	626.02	Joback Method
cpg	389.96	J/mol×K	664.83	Joback Method
cpg	404.06	J/mol×K	703.65	Joback Method
cpg	417.76	J/mol×K	742.46	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic properties of ethanol solution of chiral camphors and its derivatives:	https://www.doi.org/10.1016/j.jct.2009.05.005
Dielectric and thermodynamic study of camphor and borneol enantiomers and their binary systems:	https://www.doi.org/10.1016/j.tca.2018.04.014
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=R439662&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tt:	Triple Point Temperature
vc:	Critical Volume

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