nootkatol

Other names: 2,3,4,4a,5,6,7,8-octahydro-4,4a-dimethyl-6-(1-methylvinyl)-2-naphthol
Inchi: InChI=1S/C15H26O/c1-10(2)12-5-6-13-8-14(16)7-11(3)15(13,4)9-12/h11-14,16H,1,5-9H2
InchiKey: VHARGWWXMUPASZ-UHFFFAOYSA-N
Formula: C15H26O
SMILES: C=C(C)C1CCC2CC(O)CC(C)C2(C)C1
Mol. weight [g/mol]: 222.37
CAS: 53643-07-5

Physical Properties

Property code	Value	Unit	Source
gf	62.37	kJ/mol	Joback Method
hf	-314.34	kJ/mol	Joback Method
hfus	20.89	kJ/mol	Joback Method
hvap	63.51	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.776		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2041.91	kPa	Joback Method
rinpol	1715.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tb	648.13	K	Joback Method
tc	853.75	K	Joback Method
tf	336.89	K	Joback Method
vc	0.753	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.16	J/mol×K	648.13	Joback Method
cpg	619.17	J/mol×K	682.40	Joback Method
cpg	639.08	J/mol×K	716.67	Joback Method
cpg	658.00	J/mol×K	750.94	Joback Method
cpg	676.06	J/mol×K	785.21	Joback Method
cpg	693.38	J/mol×K	819.48	Joback Method

cpg	710.06	J/mol×K	853.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C53643075&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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
vc:	Critical Volume