Hedycariol

Inchi: InChI=1S/C15H26O/c1-12-6-5-7-13(2)9-11-14(10-8-12)15(3,4)16/h6,9,14,16H,5,7-8,10-1
InchiKey: SDMLCXJKAYFHQM-AAVBEOHCSA-N
Formula: C15H26O
SMILES: CC1=CCC(C(C)(C)O)CCC(C)=CCC1
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	-41.85	kJ/mol	Joback Method
hf	-391.61	kJ/mol	Joback Method
hfus	16.38	kJ/mol	Joback Method
hvap	67.39	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.230		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	1671.00		NIST Webbook
tb	676.46	K	Joback Method
tc	889.94	K	Joback Method
tf	341.91	K	Joback Method
vc	0.756	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.21	J/mol×K	676.46	Joback Method
cpg	619.44	J/mol×K	712.04	Joback Method
cpg	638.35	J/mol×K	747.62	Joback Method
cpg	655.96	J/mol×K	783.20	Joback Method
cpg	672.31	J/mol×K	818.78	Joback Method
cpg	687.41	J/mol×K	854.36	Joback Method
cpg	701.30	J/mol×K	889.94	Joback Method
dvisc	0.0069347	Pa×s	341.91	Joback Method
dvisc	0.0011570	Pa×s	397.67	Joback Method

dvisc	0.0002998	Pa×s	453.43	Joback Method
dvisc	0.0001044	Pa×s	509.19	Joback Method
dvisc	0.0000448	Pa×s	564.94	Joback Method
dvisc	0.0000224	Pa×s	620.70	Joback Method
dvisc	0.0000125	Pa×s	676.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326368&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
dvisc:	Dynamic viscosity
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