14-hydroxy-calamenene

Inchi: InChI=1S/C15H22O/c1-10-4-6-13-11(2)5-7-14(12(3)9-16)15(13)8-10/h4,6,8,11-12,14,16H
InchiKey: SGUPEDLSWUIQIJ-SOGVLRHJSA-N
Formula: C15H22O
SMILES: Cc1ccc2c(c1)C(C(C)CO)CCC2C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	70.25	kJ/mol	Joback Method
hf	-250.55	kJ/mol	Joback Method
hfus	25.54	kJ/mol	Joback Method
hvap	68.65	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	3.604		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
ripol	2694.00		NIST Webbook
ripol	2694.00		NIST Webbook
tb	677.32	K	Joback Method
tc	880.91	K	Joback Method
tf	366.27	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.83	J/mol×K	677.32	Joback Method
cpg	567.70	J/mol×K	711.25	Joback Method
cpg	583.59	J/mol×K	745.18	Joback Method
cpg	598.53	J/mol×K	779.11	Joback Method
cpg	612.58	J/mol×K	813.04	Joback Method
cpg	625.78	J/mol×K	846.98	Joback Method
cpg	638.18	J/mol×K	880.91	Joback Method
dvisc	0.0033634	Pa×s	366.27	Joback Method

dvisc	0.0012769	Pa×s	418.11	Joback Method
dvisc	0.0006003	Pa×s	469.95	Joback Method
dvisc	0.0003278	Pa×s	521.80	Joback Method
dvisc	0.0001997	Pa×s	573.64	Joback Method
dvisc	0.0001321	Pa×s	625.48	Joback Method
dvisc	0.0000931	Pa×s	677.32	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R338920&Units=SI

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume