Calamenen-9-ol

Inchi: InChI=1S/C15H22O/c1-9(2)15-13-7-10(3)5-6-12(13)11(4)8-14(15)16/h5-7,9,11,14-16H,8
InchiKey: HTPALWBCPQXQBN-QTWGFKIWSA-N
Formula: C15H22O
SMILES: Cc1ccc2c(c1)C(C(C)C)C(O)CC2C
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	62.54	kJ/mol	Joback Method
hf	-270.89	kJ/mol	Joback Method
hfus	26.61	kJ/mol	Joback Method
hvap	68.34	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.603		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	672.65	K	Joback Method
tc	876.14	K	Joback Method
tf	362.03	K	Joback Method
vc	0.728	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.03	J/mol×K	672.65	Joback Method
cpg	570.37	J/mol×K	706.56	Joback Method
cpg	586.70	J/mol×K	740.48	Joback Method
cpg	602.07	J/mol×K	774.39	Joback Method
cpg	616.51	J/mol×K	808.31	Joback Method
cpg	630.07	J/mol×K	842.22	Joback Method
cpg	642.78	J/mol×K	876.14	Joback Method
dvisc	0.0031559	Pa×s	362.03	Joback Method

dvisc	0.0012791	Pa×s	413.80	Joback Method
dvisc	0.0006338	Pa×s	465.57	Joback Method
dvisc	0.0003614	Pa×s	517.34	Joback Method
dvisc	0.0002283	Pa×s	569.11	Joback Method
dvisc	0.0001556	Pa×s	620.88	Joback Method
dvisc	0.0001126	Pa×s	672.65	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=R589049&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume