10«beta»-Hydroxycalamenene

Inchi: InChI=1S/C14H20O/c1-10(2)11-8-9-14(3,15)13-7-5-4-6-12(11)13/h4-7,10-11,15H,8-9H2,
InchiKey: AHVLIYTXCGGTNY-BXUZGUMPSA-N
Formula: C14H20O
SMILES: CC(C)C1CCC(C)(O)c2ccccc21
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	65.97	kJ/mol	Joback Method
hf	-203.20	kJ/mol	Joback Method
hfus	17.04	kJ/mol	Joback Method
hvap	64.61	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.427		Crippen Method
mcvol	179.370	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1649.00		NIST Webbook
ripol	2360.00		NIST Webbook
tb	649.70	K	Joback Method
tc	862.41	K	Joback Method
tf	366.38	K	Joback Method
vc	0.670	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.67	J/mol×K	649.70	Joback Method
cpg	511.18	J/mol×K	685.15	Joback Method
cpg	526.80	J/mol×K	720.60	Joback Method
cpg	541.69	J/mol×K	756.06	Joback Method
cpg	555.96	J/mol×K	791.51	Joback Method
cpg	569.76	J/mol×K	826.96	Joback Method
cpg	583.22	J/mol×K	862.41	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=R229415&Units=SI

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
vc:	Critical Volume