Cubeban-11-ol

Other names: Cubeb-11-ol
Inchi: InChI=1S/C15H26O/c1-9-7-8-15-10(2)5-6-11(14(3,4)16)13(15)12(9)15/h9-13,16H,5-8H2,
InchiKey: UDKJLEWHLZPFOR-OSDIFYQBSA-N
Formula: C15H26O
SMILES: CC1CCC23C(C)CCC(C(C)(C)O)C2C13
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	82.97	kJ/mol	Joback Method
hf	-347.45	kJ/mol	Joback Method
hfus	20.50	kJ/mol	Joback Method
hvap	62.20	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.466		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	1588.00		NIST Webbook
tb	642.27	K	Joback Method
tc	846.03	K	Joback Method
tf	383.53	K	Joback Method
vc	0.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.23	J/mol×K	642.27	Joback Method
cpg	622.35	J/mol×K	676.23	Joback Method
cpg	641.34	J/mol×K	710.19	Joback Method
cpg	659.37	J/mol×K	744.15	Joback Method
cpg	676.59	J/mol×K	778.11	Joback Method
cpg	693.20	J/mol×K	812.07	Joback Method
cpg	709.35	J/mol×K	846.03	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=R228596&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume