

4-epi-Cubebol

Inchi: InChI=1S/C15H26O/c1-9(2)11-6-5-10(3)15-8-7-14(4,16)13(15)12(11)15/h9-13,16H,5-8H
InchiKey: KONGRWVLXLWGDV-HFLBYBBMSA-N
Formula: C15H26O
SMILES: CC(C)C1CCC(C)C23CCC(C)(O)C2C13
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	72.20	kJ/mol	Joback Method
hf	-328.74	kJ/mol	Joback Method
hfus	18.09	kJ/mol	Joback Method
hvap	61.96	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.466		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2159.31	kPa	Joback Method
rinpol	1493.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1489.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1491.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1507.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1493.00		NIST Webbook
rinpol	1491.00		NIST Webbook
ripol	1956.00		NIST Webbook
ripol	1879.00		NIST Webbook
ripol	1928.00		NIST Webbook
ripol	1879.00		NIST Webbook

ripol	1956.00		NIST Webbook
ripol	1928.00		NIST Webbook
ripol	1880.00		NIST Webbook
ripol	1928.00		NIST Webbook
tb	645.30	K	Joback Method
tc	849.11	K	Joback Method
tf	390.01	K	Joback Method
vc	0.745	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.91	J/mol×K	645.30	Joback Method
cpg	616.48	J/mol×K	679.27	Joback Method
cpg	635.16	J/mol×K	713.24	Joback Method
cpg	653.15	J/mol×K	747.21	Joback Method
cpg	670.70	J/mol×K	781.17	Joback Method
cpg	688.01	J/mol×K	815.14	Joback Method
cpg	705.32	J/mol×K	849.11	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R201180&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
ripol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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