10-epi-Cubebol

Inchi:	InChI=1S/C15H24O/c1-9(2)11-6-5-10(3)15-8-7-14(4,16)13(15)12(11)15/h5-6,9-13,16H,7
InchiKey:	LMCRYOCEDDKMQA-ZRGDOOIKSA-N
Formula:	C15H24O
SMILES:	CC(C)C1C=CC(C)C23CCC(C)(O)C2C13
Mol. weight [g/mol]:	220.35
CAS:	176589-53-0

Physical Properties

Property code	Value	Unit	Source
gf	102.16	kJ/mol	Joback Method
hf	-270.96	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	62.25	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.242		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1545.00		NIST Webbook
ripol	1899.00		NIST Webbook
ripol	1899.00		NIST Webbook
tb	644.46	K	Joback Method
tc	849.94	K	Joback Method
tf	390.77	K	Joback Method
vc	0.731	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.51	J/mol×K	644.46	Joback Method
cpg	593.11	J/mol×K	678.71	Joback Method
cpg	610.85	J/mol×K	712.95	Joback Method

cpg	627.94	J/mol×K	747.20	Joback Method
cpg	644.63	J/mol×K	781.45	Joback Method
cpg	661.14	J/mol×K	815.69	Joback Method
cpg	677.70	J/mol×K	849.94	Joback Method

Sources

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=C176589530&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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