(3S,3aR,3bR,4S,7R,7aR)-4-Isopropyl-3,7-dimethylo

Other names: 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,5-8H2
InchiKey: KONGRWVLXLWGDV-UHFFFAOYSA-N
Formula: C15H26O
SMILES: CC(C)C1CCC(C)C23CCC(C)(O)C2C13
Mol. weight [g/mol]: 222.37
CAS: 23445-02-5

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	1513.00		NIST Webbook
rinpol	1511.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1513.00		NIST Webbook
rinpol	1515.00		NIST Webbook
rinpol	1518.00		NIST Webbook
rinpol	1529.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1488.00		NIST Webbook
rinpol	1512.00		NIST Webbook
rinpol	1510.00		NIST Webbook
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rinpol	1510.00	NIST Webbook
rinpol	1527.00	NIST Webbook
ripol	1914.00	NIST Webbook
ripol	1951.00	NIST Webbook
ripol	1927.00	NIST Webbook
ripol	1928.00	NIST Webbook
ripol	1957.00	NIST Webbook
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ripol	1964.00		NIST Webbook
ripol	1957.00		NIST Webbook
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ripol	1957.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1957.00		NIST Webbook
ripol	1914.00		NIST Webbook
ripol	1957.00		NIST Webbook
tb	645.30	K	Joback Method
tc	849.11	K	Joback Method
tf	390.01	K	Joback Method
vc	0.745	m3/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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23445025&Units=SI
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

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