

Isocyperol

Inchi:	InChI=1S/C15H24O/c1-10(2)12-5-7-15(4)8-6-14(16)11(3)13(15)9-12/h12-14,16H,1,3,5-9
InchiKey:	CZFHAODYOVXPIQ-AVOUXACISA-N
Formula:	C15H24O
SMILES:	C=C(C)C1CCC2(C)CCC(O)C(=C)C2C1
Mol. weight [g/mol]:	220.35

Physical Properties

Property code	Value	Unit	Source
gf	123.16	kJ/mol	Joback Method
hf	-209.76	kJ/mol	Joback Method
hfus	18.66	kJ/mol	Joback Method
hvap	63.98	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1593.00		NIST Webbook
rinpol	1593.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1590.00		NIST Webbook
tb	651.96	K	Joback Method
tc	859.17	K	Joback Method
tf	354.81	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.06	J/molxK	651.96	Joback Method
cpg	592.62	J/molxK	686.50	Joback Method
cpg	611.16	J/molxK	721.03	Joback Method
cpg	628.80	J/molxK	755.57	Joback Method
cpg	645.67	J/molxK	790.10	Joback Method
cpg	661.88	J/molxK	824.64	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=R621044&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

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