

Isocalamendiol

Inchi:	InChI=1S/C15H26O2/c1-10(2)12-7-8-14(4,16)13-6-5-11(3)9-15(12,13)17/h10,12-13,16-1
InchiKey:	AHNGXHRYPFGQWSL-UHFFFAOYSA-N
Formula:	C15H26O2
SMILES:	C=C1CCC2C(C)(O)CCC(C(C)C)C2(O)C1
Mol. weight [g/mol]:	238.37

Physical Properties

Property code	Value	Unit	Source
gf	-100.88	kJ/mol	Joback Method
hf	-467.67	kJ/mol	Joback Method
hfus	15.52	kJ/mol	Joback Method
hvap	79.71	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.891		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
ripol	1728.00		NIST Webbook
ripol	1728.00		NIST Webbook
ripol	1730.00		NIST Webbook
ripol	1730.00		NIST Webbook
ripol	2500.00		NIST Webbook
ripol	2500.00		NIST Webbook
ripol	2462.00		NIST Webbook
ripol	2462.00		NIST Webbook
tb	747.38	K	Joback Method
tc	947.43	K	Joback Method
tf	440.25	K	Joback Method
vc	0.767	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.10	J/molxK	747.38	Joback Method
cpg	679.55	J/molxK	780.72	Joback Method

cpg	696.66	J/mol×K	814.06	Joback Method
cpg	713.60	J/mol×K	847.40	Joback Method
cpg	730.54	J/mol×K	880.75	Joback Method
cpg	747.65	J/mol×K	914.09	Joback Method
cpg	765.10	J/mol×K	947.43	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=U360302&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
rinpola:	Non-polar retention indices
ripola:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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