

Isocalamenediol

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:	<chem>C=C1CCC2C(C)(O)CCC(C(C)C)C2(O)C1</chem>
Mol. weight [g/mol]:	238.37
CAS:	25330-21-6

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
mvol	207.930	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	1760.80		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/molxK	814.06	Joback Method
cpg	713.60	J/molxK	847.40	Joback Method
cpg	730.54	J/molxK	880.75	Joback Method
cpg	747.65	J/molxK	914.09	Joback Method
cpg	765.10	J/molxK	947.43	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C25330216&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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