Dehydroxy isocalamenediol

Inchi: InChI=1S/C15H24O/c1-10(2)12-7-8-15(4,16)14-6-5-11(3)9-13(12)14/h9-10,12,14,16H,3,5
InchiKey: QJUDGHWOYGNMLW-XSDATEAUSA-N
Formula: C15H24O
SMILES: C=C1C=C2C(C(C)C)CCC(C)(O)C2CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	69.47	kJ/mol	Joback Method
hf	-264.03	kJ/mol	Joback Method
hfus	17.49	kJ/mol	Joback Method
hvap	65.44	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.696		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2171.40	kPa	Joback Method
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	663.77	K	Joback Method
tc	870.50	K	Joback Method
tf	373.05	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	572.06	J/mol×K	663.77	Joback Method
cpg	590.64	J/mol×K	698.22	Joback Method
cpg	608.29	J/mol×K	732.68	Joback Method
cpg	625.13	J/mol×K	767.13	Joback Method
cpg	641.29	J/mol×K	801.59	Joback Method
cpg	656.87	J/mol×K	836.04	Joback Method
cpg	671.99	J/mol×K	870.50	Joback Method

Sources

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=R324773&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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