

«alpha»-Chenopodiol

Inchi:	InChI=1S/C15H26O2/c1-10-6-5-8-15(4)9-7-11(14(2,3)17)13(16)12(10)15/h6,11-13,16-17
InchiKey:	LBZDGNDASDARLL-UHFFFAOYSA-N
Formula:	C15H26O2
SMILES:	CC1=CCCC2(C)CCC(C(C)(C)O)C(O)C12
Mol. weight [g/mol]:	238.37
CAS:	67996-31-0

Physical Properties

Property code	Value	Unit	Source
gf	-122.86	kJ/mol	Joback Method
hf	-524.31	kJ/mol	Joback Method
hfus	19.92	kJ/mol	Joback Method
hvap	80.74	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.891		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	2278.41	kPa	Joback Method
rinpol	1855.00		NIST Webbook
rinpol	1855.00		NIST Webbook
tb	749.33	K	Joback Method
tc	950.18	K	Joback Method
tf	433.37	K	Joback Method
vc	0.766	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.65	J/mol×K	749.33	Joback Method
cpg	685.68	J/mol×K	782.81	Joback Method
cpg	702.01	J/mol×K	816.28	Joback Method
cpg	717.78	J/mol×K	849.76	Joback Method
cpg	733.11	J/mol×K	883.23	Joback Method
cpg	748.12	J/mol×K	916.71	Joback Method
cpg	762.93	J/mol×K	950.18	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C67996310&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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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