3,7-dimethyl-2(Z),6(E)-octadiene-1,8-diol

Other names: (E) 8-hydroxynerol
Inchi: InChI=1S/C10H18O2/c1-9(6-7-11)4-3-5-10(2)8-12/h5-6,11-12H,3-4,7-8H2,1-2H3/b9-6-,1
InchiKey: PREUOUJFXMCMSJ-SCWCTGRGSA-N
Formula: C10H18O2
SMILES: CC(=CCCC(C)=CCO)CO
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-96.98	kJ/mol	Joback Method
hf	-339.33	kJ/mol	Joback Method
hfus	27.62	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-2.24		Crippen Method
logp	1.644		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2829.33	kPa	Joback Method
ripol	2606.00		NIST Webbook
ripol	2613.00		NIST Webbook
ripol	2585.00		NIST Webbook
ripol	2600.00		NIST Webbook
tb	620.64	K	Joback Method
tc	791.70	K	Joback Method
tf	286.02	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.38	J/mol×K	620.64	Joback Method
cpg	410.17	J/mol×K	649.15	Joback Method
cpg	420.45	J/mol×K	677.66	Joback Method
cpg	430.24	J/mol×K	706.17	Joback Method
cpg	439.60	J/mol×K	734.68	Joback Method

cpg	448.53	J/mol×K	763.19	Joback Method
cpg	457.08	J/mol×K	791.70	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=R318991&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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