3,7-dimethyl-2,6-octaden-1,4-diol

Inchi: InChI=1S/C10H18O2/c1-8(2)4-5-10(12)9(3)6-7-11/h4,6,10-12H,5,7H2,1-3H3/b9-6+
InchiKey: PTCYLOJKSMVJTR-RMKNXTFCSA-N
Formula: C10H18O2
SMILES: CC(C)=CCC(O)C(C)=CCO
Mol. weight [g/mol]: 170.25

Physical Properties

Property code	Value	Unit	Source
gf	-99.42	kJ/mol	Joback Method
hf	-344.61	kJ/mol	Joback Method
hfus	24.09	kJ/mol	Joback Method
hvap	70.90	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	1.642		Crippen Method
mcvol	154.900	ml/mol	McGowan Method
pc	2853.57	kPa	Joback Method
ripol	2472.00		NIST Webbook
ripol	2469.00		NIST Webbook
ripol	2469.00		NIST Webbook
tb	620.20	K	Joback Method
tc	793.87	K	Joback Method
tf	271.02	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	399.85	J/mol×K	620.20	Joback Method
cpg	410.84	J/mol×K	649.14	Joback Method
cpg	421.30	J/mol×K	678.09	Joback Method
cpg	431.26	J/mol×K	707.03	Joback Method
cpg	440.76	J/mol×K	735.98	Joback Method
cpg	449.81	J/mol×K	764.92	Joback Method
cpg	458.47	J/mol×K	793.87	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=R334473&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume