4,6-Decadiyne-3,8-diol, 3,8-dimethyl-

Other names: 3,8-Dimethyl-4,6-decadiyne-3,8-diol
Inchi: InChI=1S/C12H18O2/c1-5-11(3,13)9-7-8-10-12(4,14)6-2/h13-14H,5-6H2,1-4H3
InchiKey: GLWDRGVPXZBLDS-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: CCC(C)(O)C#CC#CC(C)(O)CC
Mol. weight [g/mol]: 194.27
CAS: 6626-33-1

Physical Properties

Property code	Value	Unit	Source
gf	187.80	kJ/mol	Joback Method
hf	-68.37	kJ/mol	Joback Method
hfus	26.43	kJ/mol	Joback Method
hvap	77.38	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	1.315		Crippen Method
mcvol	174.480	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	669.86	K	Joback Method
tc	871.11	K	Joback Method
tf	563.68	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.39	J/mol×K	669.86	Joback Method
cpg	475.32	J/mol×K	703.40	Joback Method
cpg	486.54	J/mol×K	736.94	Joback Method
cpg	497.11	J/mol×K	770.48	Joback Method
cpg	507.08	J/mol×K	804.02	Joback Method
cpg	516.52	J/mol×K	837.56	Joback Method
cpg	525.47	J/mol×K	871.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6626331&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume