2,7-Dimethyloctadiyne-3,5-diol-2,7

Other names: 2,7-Dimethyl-octa-3,5-diyne-2,7-diol
3,5-Octadiyne-2,7-diol, 2,7-dimethyl-
Inchi: InChI=1S/C10H14O2/c1-9(2,11)7-5-6-8-10(3,4)12/h11-12H,1-4H3
InchiKey: CKVWIEREOYIKNC-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: CC(C)(O)C#CC#CC(C)(C)O
Mol. weight [g/mol]: 166.22
CAS: 5929-72-6

Physical Properties

Property code	Value	Unit	Source
gf	170.96	kJ/mol	Joback Method
hf	-27.09	kJ/mol	Joback Method
hfus	21.25	kJ/mol	Joback Method
hvap	72.92	kJ/mol	Joback Method
log10ws	-2.35		Crippen Method
logp	0.535		Crippen Method
mcvol	146.300	ml/mol	McGowan Method
pc	3736.23	kPa	Joback Method
tb	624.10	K	Joback Method
tc	831.01	K	Joback Method
tf	541.14	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	365.70	J/mol×K	624.10	Joback Method
cpg	376.29	J/mol×K	658.58	Joback Method
cpg	386.20	J/mol×K	693.07	Joback Method
cpg	395.48	J/mol×K	727.55	Joback Method
cpg	404.19	J/mol×K	762.04	Joback Method
cpg	412.38	J/mol×K	796.52	Joback Method
cpg	420.12	J/mol×K	831.01	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=C5929726&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume