2,4-Hexadiyne-1,6-diol

Other names:	2,4-Hexadiyn-1,6-diol
	Diacetylene glycol
	2,4-Hexadiynediol
	hexa-2,4-diyne-1,6-diol
Inchi:	InChI=1S/C6H6O2/c7-5-3-1-2-4-6-8/h7-8H,5-6H2
InchiKey:	JXMQYKBAZRDVTC-UHFFFAOYSA-N
Formula:	C6H6O2
SMILES:	OCC#CC#CCO
Mol. weight [g/mol]:	110.11
CAS:	3031-68-3

Physical Properties

Property code	Value	Unit	Source
gf	131.60	kJ/mol	Joback Method
hf	72.97	kJ/mol	Joback Method
hfus	25.72	kJ/mol	Joback Method
hvap	66.61	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	-1.022		Crippen Method
mcvol	89.940	ml/mol	McGowan Method
pc	6009.25	kPa	Joback Method
tb	539.04	K	Joback Method
tc	734.81	K	Joback Method
tf	491.22	K	Joback Method
vc	0.334	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.46	J/mol×K	539.04	Joback Method
cpg	187.27	J/mol×K	571.67	Joback Method
cpg	192.85	J/mol×K	604.30	Joback Method
cpg	198.18	J/mol×K	636.93	Joback Method
cpg	203.29	J/mol×K	669.56	Joback Method

cpg	208.18	J/mol×K	702.18	Joback Method
cpg	212.85	J/mol×K	734.81	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=C3031683&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