Dodec-5-yne-1,4-diol

Inchi: InChI=1S/C12H22O2/c1-2-3-4-5-6-7-9-12(14)10-8-11-13/h12-14H,2-6,8,10-11H2,1H3
InchiKey: PYYUDKGZNALMSY-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CCCCCCC#CC(O)CCCO
Mol. weight [g/mol]: 198.30

Physical Properties

Property code	Value	Unit	Source
gf	-23.12	kJ/mol	Joback Method
hf	-328.45	kJ/mol	Joback Method
hfus	34.61	kJ/mol	Joback Method
hvap	77.43	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.094		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1699.00		NIST Webbook
tb	666.88	K	Joback Method
tc	839.13	K	Joback Method
tf	437.74	K	Joback Method
vc	0.702	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.85	J/mol×K	666.88	Joback Method
cpg	514.19	J/mol×K	695.59	Joback Method
cpg	525.99	J/mol×K	724.30	Joback Method
cpg	537.26	J/mol×K	753.01	Joback Method
cpg	548.02	J/mol×K	781.72	Joback Method
cpg	558.29	J/mol×K	810.42	Joback Method
cpg	568.10	J/mol×K	839.13	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=R412969&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume