5,7-Dodecadiyn-1,12-diol

Inchi: InChI=1S/C12H18O2/c13-11-9-7-5-3-1-2-4-6-8-10-12-14/h13-14H,5-12H2
InchiKey: SEWYHOMCDKWYEF-UHFFFAOYSA-N
Formula: C12H18O2
SMILES: OCCCCC#CC#CCCCCO
Mol. weight [g/mol]: 194.27
CAS: 74602-32-7

Physical Properties

Property code	Value	Unit	Source
gf	182.12	kJ/mol	Joback Method
hf	-50.87	kJ/mol	Joback Method
hfus	41.26	kJ/mol	Joback Method
hvap	79.97	kJ/mol	Joback Method
log10ws	-2.96		Crippen Method
logp	1.318		Crippen Method
mcvol	174.480	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1724.00		NIST Webbook
rinpol	1724.00		NIST Webbook
tb	676.32	K	Joback Method
tc	860.30	K	Joback Method
tf	558.84	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	457.16	J/mol×K	676.32	Joback Method
cpg	468.49	J/mol×K	706.98	Joback Method
cpg	479.31	J/mol×K	737.65	Joback Method
cpg	489.63	J/mol×K	768.31	Joback Method
cpg	499.47	J/mol×K	798.97	Joback Method
cpg	508.86	J/mol×K	829.63	Joback Method
cpg	517.80	J/mol×K	860.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74602327&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume