4-Hydroxy-1-(2-tetrahydropyranyloxy)dodec-5-yne

Inchi: InChI=1S/C17H30O3/c1-2-3-4-5-6-7-11-16(18)12-10-15-20-17-13-8-9-14-19-17/h16-18H
InchiKey: VPAKFIVPDQNHIO-UHFFFAOYSA-N
Formula: C17H30O3
SMILES: CCCCCCC#CC(O)CCCOC1CCCCO1
Mol. weight [g/mol]: 282.42

Physical Properties

Property code	Value	Unit	Source
gf	-10.87	kJ/mol	Joback Method
hf	-489.32	kJ/mol	Joback Method
hfus	44.47	kJ/mol	Joback Method
hvap	79.23	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.645		Crippen Method
mcvol	248.540	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2141.00		NIST Webbook
rinpol	2141.00		NIST Webbook
tb	758.02	K	Joback Method
tc	952.17	K	Joback Method
tf	489.45	K	Joback Method
vc	0.934	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.79	J/mol×K	758.02	Joback Method
cpg	785.71	J/mol×K	790.38	Joback Method
cpg	802.59	J/mol×K	822.74	Joback Method
cpg	818.44	J/mol×K	855.09	Joback Method
cpg	833.30	J/mol×K	887.45	Joback Method
cpg	847.18	J/mol×K	919.81	Joback Method
cpg	860.12	J/mol×K	952.17	Joback Method

Sources

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=R412949&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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