

2,2-Bis(hydroxymethyl)-2,2',2''-nitrilotriethanol, pentaethyl ether

Other names: 2-[Bis(2-hydroxyethyl)amino]-2-(hydroxymethyl)propane-1,3-diol, pentaethyl ether
1,3-Diethoxy-N,N-bis(2-ethoxyethyl)-2-(ethoxymethyl)propan-2-amine

Inchi: InChI=1S/C18H39NO5/c1-6-20-13-11-19(12-14-21-7-2)18(15-22-8-3,16-23-9-4)17-24-10
InchiKey: VXAAHGJNAGTIOV-UHFFFAOYSA-N
Formula: C18H39NO5
SMILES: CCOCCN(CCOCC)C(COCC)(COCC)COCC
Mol. weight [g/mol]: 349.51

Physical Properties

Property code	Value	Unit	Source
gf	-310.70	kJ/mol	Joback Method
hf	-1017.17	kJ/mol	Joback Method
hfus	43.92	kJ/mol	Joback Method
hvap	68.46	kJ/mol	Joback Method
log10ws	-1.48		Crippen Method
logp	2.210		Crippen Method
mcvol	303.810	ml/mol	McGowan Method
pc	1100.81	kPa	Joback Method
rinpol	1841.00		NIST Webbook
tb	732.55	K	Joback Method
tc	903.51	K	Joback Method
tf	438.66	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	933.38	J/molxK	732.55	Joback Method
cpg	953.01	J/molxK	761.04	Joback Method
cpg	971.67	J/molxK	789.54	Joback Method
cpg	989.36	J/molxK	818.03	Joback Method
cpg	1006.10	J/molxK	846.52	Joback Method
cpg	1021.88	J/molxK	875.01	Joback Method
cpg	1036.71	J/molxK	903.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U378704&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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