2-Diethylamino-2-methylpropane-1,3-diol, diethyl ether

Other names: 1,3-Diethoxy-N,N-diethyl-2-methylpropan-2-amine
Inchi: InChI=1S/C12H27NO2/c1-6-13(7-2)12(5,10-14-8-3)11-15-9-4/h6-11H2,1-5H3
InchiKey: LKZXROCDPXMPFZ-UHFFFAOYSA-N
Formula: C12H27NO2
SMILES: CCOCC(C)(COCC)N(CC)CC
Mol. weight [g/mol]: 217.35

Physical Properties

Property code	Value	Unit	Source
gf	-46.22	kJ/mol	Joback Method
hf	-496.67	kJ/mol	Joback Method
hfus	24.82	kJ/mol	Joback Method
hvap	47.87	kJ/mol	Joback Method
log10ws	-1.70		Crippen Method
logp	2.160		Crippen Method
mcvol	201.660	ml/mol	McGowan Method
pc	1755.07	kPa	Joback Method
rinpol	1239.00		NIST Webbook
rinpol	1239.00		NIST Webbook
tb	528.01	K	Joback Method
tc	696.09	K	Joback Method
tf	304.35	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	503.48	J/mol×K	528.01	Joback Method
cpg	521.23	J/mol×K	556.02	Joback Method
cpg	538.23	J/mol×K	584.04	Joback Method
cpg	554.51	J/mol×K	612.05	Joback Method
cpg	570.08	J/mol×K	640.07	Joback Method
cpg	584.97	J/mol×K	668.08	Joback Method
cpg	599.18	J/mol×K	696.09	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=U378724&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume