

2-[Bis(2-hydroxyethyl)amino]-2-(hydroxymethyl)propan-2-amine

Other names: 1,3-Dimethoxy-N,N-bis(2-methoxyethyl)-2-(methoxymethyl)propan-2-amine
InChI: InChI=1S/C13H29NO5/c1-15-8-6-14(7-9-16-2)13(10-17-3,11-18-4)12-19-5/h6-12H2,1-5H1
InchiKey: OKACOZYDHFYGAS-UHFFFAOYSA-N
Formula: C13H29NO5
SMILES: COCCN(CCOC)C(COC)(COC)COC
Mol. weight [g/mol]: 279.37

Physical Properties

Property code	Value	Unit	Source
gf	-352.80	kJ/mol	Joback Method
hf	-913.97	kJ/mol	Joback Method
hfus	30.97	kJ/mol	Joback Method
hvap	57.33	kJ/mol	Joback Method
log10ws	0.62		Crippen Method
logp	0.259		Crippen Method
mcvol	233.360	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinpol	1640.00		NIST Webbook
tb	618.15	K	Joback Method
tc	785.26	K	Joback Method
tf	382.31	K	Joback Method
vc	0.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.51	J/mol×K	618.15	Joback Method
cpg	662.92	J/mol×K	646.00	Joback Method
cpg	679.64	J/mol×K	673.85	Joback Method
cpg	695.64	J/mol×K	701.71	Joback Method
cpg	710.94	J/mol×K	729.56	Joback Method
cpg	725.52	J/mol×K	757.41	Joback Method
cpg	739.39	J/mol×K	785.26	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=U378705&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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