2-[Bis(2-methyloxyethyl)amino]acetic acid, methyl ester

Other names: Methyl 2-[bis(2-methoxyethyl)amino]acetate
Inchi: InChI=1S/C9H19NO4/c1-12-6-4-10(5-7-13-2)8-9(11)14-3/h4-8H2,1-3H3
InchiKey: LDURYHFKBFBINS-UHFFFAOYSA-N
Formula: C9H19NO4
SMILES: COCCN(CCOC)CC(=O)OC
Mol. weight [g/mol]: 205.25

Physical Properties

Property code	Value	Unit	Source
gf	-308.24	kJ/mol	Joback Method
hf	-670.80	kJ/mol	Joback Method
hfus	27.25	kJ/mol	Joback Method
hvap	51.65	kJ/mol	Joback Method
log10ws	0.80		Crippen Method
logp	-0.246		Crippen Method
mcvol	166.830	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1356.00		NIST Webbook
rinpol	1356.00		NIST Webbook
tb	538.89	K	Joback Method
tc	709.99	K	Joback Method
tf	340.28	K	Joback Method
vc	0.618	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	408.10	J/mol×K	538.89	Joback Method
cpg	421.71	J/mol×K	567.41	Joback Method
cpg	434.85	J/mol×K	595.92	Joback Method
cpg	447.50	J/mol×K	624.44	Joback Method
cpg	459.66	J/mol×K	652.95	Joback Method
cpg	471.33	J/mol×K	681.47	Joback Method
cpg	482.49	J/mol×K	709.99	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=U378708&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