

Ethyl 2-[bis(2-ethoxyethyl)amino]acetate

Other names:	2-[Bis(2-ethoxyethyl)amino]acetic acid, ethyl ester
Inchi:	InChI=1S/C12H25NO4/c1-4-15-9-7-13(8-10-16-5-2)11-12(14)17-6-3/h4-11H2,1-3H3
InchiKey:	WIVGKIJWHFVGJU-UHFFFAOYSA-N
Formula:	C12H25NO4
SMILES:	CCOCCN(CCOCC)CC(=O)OCC
Mol. weight [g/mol]:	247.33

Physical Properties

Property code	Value	Unit	Source
gf	-282.98	kJ/mol	Joback Method
hf	-732.72	kJ/mol	Joback Method
hfus	35.02	kJ/mol	Joback Method
hvap	58.33	kJ/mol	Joback Method
log10ws	-0.45		Crippen Method
logp	0.925		Crippen Method
mcvol	209.100	ml/mol	McGowan Method
pc	1795.46	kPa	Joback Method
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
tb	607.53	K	Joback Method
tc	775.84	K	Joback Method
tf	374.09	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.25	J/molxK	607.53	Joback Method
cpg	573.96	J/molxK	635.58	Joback Method
cpg	589.06	J/molxK	663.63	Joback Method
cpg	603.52	J/molxK	691.69	Joback Method
cpg	617.36	J/molxK	719.74	Joback Method
cpg	630.56	J/molxK	747.79	Joback Method
cpg	643.14	J/molxK	775.84	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=U378721&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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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