2,2'-(2-Amino-2-oxoethylazanediyl)diacetic acid, dimethyl ester

Other names: Dimethyl 2,2'-[(2-amino-2-oxoethyl)azanediyl]diacetate
Inchi: InChI=1S/C8H14N2O5/c1-14-7(12)4-10(3-6(9)11)5-8(13)15-2/h3-5H2,1-2H3,(H2,9,11)
InchiKey: BUZJDEDDXIPFQR-UHFFFAOYSA-N
Formula: C8H14N2O5
SMILES: COC(=O)CN(CC(N)=O)CC(=O)OC
Mol. weight [g/mol]: 218.21

Physical Properties

Property code	Value	Unit	Source
gf	-403.05	kJ/mol	Joback Method
hf	-709.31	kJ/mol	Joback Method
hfus	31.87	kJ/mol	Joback Method
hvap	71.14	kJ/mol	Joback Method
log10ws	1.32		Crippen Method
logp	-1.880		Crippen Method
mcvol	159.990	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1728.00		NIST Webbook
tb	673.86	K	Joback Method
tc	871.51	K	Joback Method
tf	489.90	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	429.95	J/mol×K	673.86	Joback Method
cpg	440.94	J/mol×K	706.80	Joback Method
cpg	451.28	J/mol×K	739.74	Joback Method
cpg	460.98	J/mol×K	772.69	Joback Method
cpg	470.02	J/mol×K	805.63	Joback Method
cpg	478.41	J/mol×K	838.57	Joback Method
cpg	486.16	J/mol×K	871.51	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U378706&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
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