1,3-Di-(1,2-dicarbethoxyethyl) urea

Inchi: InChI=1S/C17H28N2O9/c1-5-25-13(20)9-11(15(22)27-7-3)18-17(24)19-12(16(23)28-8-4)
InchiKey: DTWHGRWKYRGPGN-UHFFFAOYSA-N
Formula: C17H28N2O9
SMILES: CCOC(=O)CC(NC(=O)NC(CC(=O)OCC)C(=O)OCC)C(=O)OCC
Mol. weight [g/mol]: 404.41
CAS: 116435-07-5

Physical Properties

Property code	Value	Unit	Source
gf	-798.44	kJ/mol	Joback Method
hf	-1389.61	kJ/mol	Joback Method
hfus	55.68	kJ/mol	Joback Method
hvap	108.90	kJ/mol	Joback Method
log10ws	-1.74		Crippen Method
logp	0.055		Crippen Method
mcvol	301.680	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
tb	1046.85	K	Joback Method
tc	1283.71	K	Joback Method
tf	695.24	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1002.82	J/mol×K	1046.85	Joback Method
cpg	1011.19	J/mol×K	1086.33	Joback Method
cpg	1017.56	J/mol×K	1125.80	Joback Method
cpg	1021.91	J/mol×K	1165.28	Joback Method
cpg	1024.23	J/mol×K	1204.76	Joback Method
cpg	1024.49	J/mol×K	1244.23	Joback Method
cpg	1022.67	J/mol×K	1283.71	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=C116435075&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume