1,3-Di-(1,3-dicarbethoxypropyl) urea

Inchi: InChI=1S/C19H32N2O9/c1-5-27-15(22)11-9-13(17(24)29-7-3)20-19(26)21-14(18(25)30-8
InchiKey: FIGMIPZJZUVFKC-UHFFFAOYSA-N
Formula: C19H32N2O9
SMILES: CCOC(=O)CCC(NC(=O)NC(CCC(=O)OCC)C(=O)OCC)C(=O)OCC
Mol. weight [g/mol]: 432.47
CAS: 116295-55-7

Physical Properties

Property code	Value	Unit	Source
gf	-781.60	kJ/mol	Joback Method
hf	-1430.89	kJ/mol	Joback Method
hfus	60.86	kJ/mol	Joback Method
hvap	113.35	kJ/mol	Joback Method
log10ws	-2.58		Crippen Method
logp	0.836		Crippen Method
mcvol	329.860	ml/mol	McGowan Method
pc	1319.43	kPa	Joback Method
tb	1092.61	K	Joback Method
tc	1346.71	K	Joback Method
tf	717.78	K	Joback Method
vc	1.260	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.27	J/mol×K	1092.61	Joback Method
cpg	1127.22	J/mol×K	1134.96	Joback Method
cpg	1132.74	J/mol×K	1177.31	Joback Method
cpg	1135.82	J/mol×K	1219.66	Joback Method
cpg	1136.44	J/mol×K	1262.01	Joback Method
cpg	1134.61	J/mol×K	1304.36	Joback Method
cpg	1130.29	J/mol×K	1346.71	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=C116295557&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