

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

Inchi:	InChI=1S/C11H20N2O5/c1-3-17-9(14)5-7-12-11(16)13-8-6-10(15)18-4-2/h3-8H2,1-2H3,(
InchiKey:	FWPIAOFQVJMQGP-UHFFFAOYSA-N
Formula:	C11H20N2O5
SMILES:	CCOC(=O)CCNC(=O)NCCC(=O)OCC
Mol. weight [g/mol]:	260.29
CAS:	116668-28-1

Physical Properties

Property code	Value	Unit	Source
gf	-376.24	kJ/mol	Joback Method
hf	-765.61	kJ/mol	Joback Method
hfus	41.62	kJ/mol	Joback Method
hvap	78.01	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	0.192		Crippen Method
mcvol	202.260	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
tb	757.87	K	Joback Method
tc	948.80	K	Joback Method
tf	513.30	K	Joback Method
vc	0.775	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.08	J/molxK	757.87	Joback Method
cpg	602.45	J/molxK	789.69	Joback Method
cpg	614.04	J/molxK	821.51	Joback Method
cpg	624.85	J/molxK	853.33	Joback Method
cpg	634.89	J/molxK	885.15	Joback Method
cpg	644.15	J/molxK	916.98	Joback Method
cpg	652.64	J/molxK	948.80	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=C116668281&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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