1,3-Di-(1-carbethoxy-3-methylbutyl) urea

Inchi: InChI=1S/C17H32N2O5/c1-7-23-15(20)13(9-11(3)4)18-17(22)19-14(10-12(5)6)16(21)24-
InchiKey: RJSMGWKDCUHEAZ-UHFFFAOYSA-N
Formula: C17H32N2O5
SMILES: CCOC(=O)C(CC(C)C)NC(=O)NC(CC(C)C)C(=O)OCC
Mol. weight [g/mol]: 344.45
CAS: 70779-90-7

Physical Properties

Property code	Value	Unit	Source
gf	-335.48	kJ/mol	Joback Method
hf	-910.57	kJ/mol	Joback Method
hfus	43.06	kJ/mol	Joback Method
hvap	89.81	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	2.241		Crippen Method
mcvol	286.800	ml/mol	McGowan Method
pc	1438.07	kPa	Joback Method
tb	893.39	K	Joback Method
tc	1097.13	K	Joback Method
tf	520.92	K	Joback Method
vc	1.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	934.32	J/mol×K	893.39	Joback Method
cpg	949.01	J/mol×K	927.35	Joback Method
cpg	962.48	J/mol×K	961.30	Joback Method
cpg	974.75	J/mol×K	995.26	Joback Method
cpg	985.83	J/mol×K	1029.22	Joback Method
cpg	995.74	J/mol×K	1063.17	Joback Method
cpg	1004.51	J/mol×K	1097.13	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=C70779907&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