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

Inchi: InChI=1S/C17H24N2O5/c1-3-23-15(20)11-10-14(16(21)24-4-2)19-17(22)18-12-13-8-6-5-
InchiKey: LUKOKKYTVBMHSU-UHFFFAOYSA-N
Formula: C17H24N2O5
SMILES: CCOC(=O)CCC(NC(=O)NCc1ccccc1)C(=O)OCC
Mol. weight [g/mol]: 336.38
CAS: 96977-92-3

Physical Properties

Property code	Value	Unit	Source
gf	-215.75	kJ/mol	Joback Method
hf	-658.20	kJ/mol	Joback Method
hfus	47.67	kJ/mol	Joback Method
hvap	93.25	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	1.761		Crippen Method
mcvol	263.040	ml/mol	McGowan Method
pc	1841.99	kPa	Joback Method
tb	921.39	K	Joback Method
tc	1137.29	K	Joback Method
tf	592.34	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	831.37	J/mol×K	921.39	Joback Method
cpg	843.46	J/mol×K	957.37	Joback Method
cpg	854.34	J/mol×K	993.36	Joback Method
cpg	864.05	J/mol×K	1029.34	Joback Method
cpg	872.61	J/mol×K	1065.32	Joback Method
cpg	880.04	J/mol×K	1101.31	Joback Method
cpg	886.38	J/mol×K	1137.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96977923&Units=SI
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

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