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

Inchi: InChI=1S/C16H22N2O5/c1-3-22-14(19)10-13(15(20)23-4-2)18-16(21)17-11-12-8-6-5-7-9
InchiKey: KYMIACLGFMZIJX-UHFFFAOYSA-N
Formula: C16H22N2O5
SMILES: CCOC(=O)CC(NC(=O)NCc1ccccc1)C(=O)OCC
Mol. weight [g/mol]: 322.36
CAS: 97021-39-1

Physical Properties

Property code	Value	Unit	Source
gf	-224.17	kJ/mol	Joback Method
hf	-637.56	kJ/mol	Joback Method
hfus	45.09	kJ/mol	Joback Method
hvap	91.03	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	1.371		Crippen Method
mcvol	248.950	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
tb	898.51	K	Joback Method
tc	1113.77	K	Joback Method
tf	581.07	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	773.87	J/mol×K	898.51	Joback Method
cpg	785.80	J/mol×K	934.39	Joback Method
cpg	796.57	J/mol×K	970.26	Joback Method
cpg	806.20	J/mol×K	1006.14	Joback Method
cpg	814.72	J/mol×K	1042.02	Joback Method
cpg	822.14	J/mol×K	1077.90	Joback Method
cpg	828.50	J/mol×K	1113.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C97021391&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

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