1-Benzyl-3-carbethoxymethyl urea

Inchi: InChI=1S/C12H16N2O3/c1-2-17-11(15)9-14-12(16)13-8-10-6-4-3-5-7-10/h3-7H,2,8-9H2,
InchiKey: JOGHOEBNQXZSDF-UHFFFAOYSA-N
Formula: C12H16N2O3
SMILES: CCOC(=O)CNC(=O)NCc1ccccc1
Mol. weight [g/mol]: 236.27
CAS: 91558-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-21.49	kJ/mol	Joback Method
hf	-304.92	kJ/mol	Joback Method
hfus	35.46	kJ/mol	Joback Method
hvap	73.36	kJ/mol	Joback Method
log10ws	-2.44		Crippen Method
logp	1.049		Crippen Method
mcvol	185.150	ml/mol	McGowan Method
pc	2758.46	kPa	Joback Method
tb	731.14	K	Joback Method
tc	943.47	K	Joback Method
tf	478.83	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.33	J/mol×K	731.14	Joback Method
cpg	527.18	J/mol×K	766.53	Joback Method
cpg	539.11	J/mol×K	801.92	Joback Method
cpg	550.14	J/mol×K	837.31	Joback Method
cpg	560.32	J/mol×K	872.70	Joback Method
cpg	569.66	J/mol×K	908.08	Joback Method
cpg	578.19	J/mol×K	943.47	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91558020&Units=SI

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