1-Benzyl-3-(10-carbethoxydecyl) urea

Inchi: InChI=1S/C21H34N2O3/c1-2-26-20(24)16-12-7-5-3-4-6-8-13-17-22-21(25)23-18-19-14-1
InchiKey: UYWQBUQSUNRPFQ-UHFFFAOYSA-N
Formula: C21H34N2O3
SMILES: CCOC(=O)CCCCCCCCCCNC(=O)NCc1ccccc1
Mol. weight [g/mol]: 362.51
CAS: 95001-15-3

Physical Properties

Property code	Value	Unit	Source
gf	54.29	kJ/mol	Joback Method
hf	-490.68	kJ/mol	Joback Method
hfus	58.77	kJ/mol	Joback Method
hvap	93.39	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	4.560		Crippen Method
mcvol	311.960	ml/mol	McGowan Method
pc	1305.17	kPa	Joback Method
tb	937.06	K	Joback Method
tc	1148.90	K	Joback Method
tf	580.26	K	Joback Method
vc	1.204	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1027.92	J/mol×K	937.06	Joback Method
cpg	1043.32	J/mol×K	972.37	Joback Method
cpg	1057.52	J/mol×K	1007.67	Joback Method
cpg	1070.58	J/mol×K	1042.98	Joback Method
cpg	1082.56	J/mol×K	1078.29	Joback Method
cpg	1093.51	J/mol×K	1113.59	Joback Method
cpg	1103.50	J/mol×K	1148.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C95001153&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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