n-octyl carbamate

Inchi: InChI=1S/C9H19NO2/c1-2-3-4-5-6-7-8-12-9(10)11/h2-8H2,1H3,(H2,10,11)
InchiKey: YPNZTHVEMNUDND-UHFFFAOYSA-N
Formula: C9H19NO2
SMILES: CCCCCCCCOC(N)=O
Mol. weight [g/mol]: 173.26

Physical Properties

Property code	Value	Unit	Source
gf	-142.57	kJ/mol	Joback Method
hf	-440.10	kJ/mol	Joback Method
hfus	27.05	kJ/mol	Joback Method
hvap	55.42	kJ/mol	Joback Method
log10ws	-3.30		Aqueous Solubility Prediction Method
logp	2.442		Crippen Method
mcvol	155.090	ml/mol	McGowan Method
pc	2553.34	kPa	Joback Method
tb	554.14	K	Joback Method
tc	738.11	K	Joback Method
tf	346.61	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.52	J/mol×K	554.14	Joback Method
cpg	397.99	J/mol×K	584.80	Joback Method
cpg	410.88	J/mol×K	615.46	Joback Method
cpg	423.21	J/mol×K	646.12	Joback Method
cpg	434.99	J/mol×K	676.79	Joback Method
cpg	446.21	J/mol×K	707.45	Joback Method
cpg	456.89	J/mol×K	738.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

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