1-Heptanol, carbamate

Other names: n-heptyl carbamate
Inchi: InChI=1S/C8H17NO2/c1-2-3-4-5-6-7-11-8(9)10/h2-7H2,1H3,(H2,9,10)
InchiKey: AXMPFOXRWZXZFA-UHFFFAOYSA-N
Formula: C8H17NO2
SMILES: CCCCCCCOC(N)=O
Mol. weight [g/mol]: 159.23

Physical Properties

Property code	Value	Unit	Source
gf	-150.99	kJ/mol	Joback Method
hf	-419.46	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	53.20	kJ/mol	Joback Method
log10ws	-2.62		Aqueous Solubility Prediction Method
logp	2.052		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2820.33	kPa	Joback Method
rinpol	1267.00		NIST Webbook
tb	531.26	K	Joback Method
tc	717.25	K	Joback Method
tf	335.34	K	Joback Method
vc	0.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.10	J/mol×K	531.26	Joback Method
cpg	350.72	J/mol×K	562.26	Joback Method
cpg	362.81	J/mol×K	593.26	Joback Method
cpg	374.39	J/mol×K	624.26	Joback Method
cpg	385.45	J/mol×K	655.26	Joback Method
cpg	396.00	J/mol×K	686.26	Joback Method
cpg	406.05	J/mol×K	717.25	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R579389&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume