1-Hexanol, carbamate

Other names: n-hexyl carbamate
Inchi: InChI=1S/C7H15NO2/c1-2-3-4-5-6-10-7(8)9/h2-6H2,1H3,(H2,8,9)
InchiKey: ROASJEHPZNKHOF-UHFFFAOYSA-N
Formula: C7H15NO2
SMILES: CCCCCCOC(N)=O
Mol. weight [g/mol]: 145.20

Physical Properties

Property code	Value	Unit	Source
gf	-159.41	kJ/mol	Joback Method
hf	-398.82	kJ/mol	Joback Method
hfus	21.87	kJ/mol	Joback Method
hvap	50.97	kJ/mol	Joback Method
log10ws	-1.92		Aqueous Solubility Prediction Method
logp	1.662		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	3131.49	kPa	Joback Method
rinpol	1165.00		NIST Webbook
rinpol	1165.00		NIST Webbook
tb	508.38	K	Joback Method
tc	696.51	K	Joback Method
tf	324.07	K	Joback Method
vc	0.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.56	J/mol×K	508.38	Joback Method
cpg	305.22	J/mol×K	539.73	Joback Method
cpg	316.40	J/mol×K	571.09	Joback Method
cpg	327.11	J/mol×K	602.44	Joback Method
cpg	337.36	J/mol×K	633.80	Joback Method
cpg	347.16	J/mol×K	665.15	Joback Method

cpg	356.49	J/mol×K	696.51	Joback Method

Sources

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=R579394&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume