1-Pentanol, carbamate

Other names: n-amyl carbamate
Inchi: InChI=1S/C6H13NO2/c1-2-3-4-5-9-6(7)8/h2-5H2,1H3,(H2,7,8)
InchiKey: MYDQAEQZZKVJSL-UHFFFAOYSA-N
Formula: C6H13NO2
SMILES: CCCCCOC(N)=O
Mol. weight [g/mol]: 131.17

Physical Properties

Property code	Value	Unit	Source
gf	-167.83	kJ/mol	Joback Method
hf	-378.18	kJ/mol	Joback Method
hfus	19.28	kJ/mol	Joback Method
hvap	48.75	kJ/mol	Joback Method
log10ws	-1.47		Aqueous Solubility Prediction Method
logp	1.272		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3497.14	kPa	Joback Method
rinpol	1070.00		NIST Webbook
tb	485.50	K	Joback Method
tc	675.81	K	Joback Method
tf	312.80	K	Joback Method
vc	0.424	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	251.01	J/mol×K	485.50	Joback Method
cpg	261.57	J/mol×K	517.22	Joback Method
cpg	271.73	J/mol×K	548.94	Joback Method
cpg	281.48	J/mol×K	580.65	Joback Method
cpg	290.81	J/mol×K	612.37	Joback Method
cpg	299.74	J/mol×K	644.09	Joback Method
cpg	308.26	J/mol×K	675.81	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R579418&Units=SI
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

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