Hexyl carbamate

Inchi: InChI=1S/C7H15NO2/c1-3-4-5-6-8-7(9)10-2/h3-6H2,1-2H3,(H,8,9)
InchiKey: VBJIQWCGMYVMKK-UHFFFAOYSA-N
Formula: C7H15NO2
SMILES: CCCCCNC(=O)OC
Mol. weight [g/mol]: 145.20
CAS: 2114-20-7

Physical Properties

Property code	Value	Unit	Source
gf	-136.47	kJ/mol	Joback Method
hf	-379.14	kJ/mol	Joback Method
hfus	21.77	kJ/mol	Joback Method
hvap	46.77	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.533		Crippen Method
mcvol	126.910	ml/mol	McGowan Method
pc	2982.79	kPa	Joback Method
tb	486.02	K	Joback Method
tc	665.66	K	Joback Method
tf	293.47	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	282.94	J/mol×K	486.02	Joback Method
cpg	294.66	J/mol×K	515.96	Joback Method
cpg	305.94	J/mol×K	545.90	Joback Method
cpg	316.78	J/mol×K	575.84	Joback Method
cpg	327.18	J/mol×K	605.78	Joback Method
cpg	337.15	J/mol×K	635.72	Joback Method
cpg	346.69	J/mol×K	665.66	Joback Method
hsubt	96.20 ± 0.80	kJ/mol	302.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2114207&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
hsubt:	Enthalpy of sublimation at a given temperature
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