Isobutylcarbamate, N-hexyl

Inchi: InChI=1S/C11H23NO2/c1-4-5-6-7-8-12-11(13)14-9-10(2)3/h10H,4-9H2,1-3H3,(H,12,13)
InchiKey: FTGWBFMEPQSPAF-UHFFFAOYSA-N
Formula: C11H23NO2
SMILES: CCCCCCNC(=O)OCC(C)C
Mol. weight [g/mol]: 201.31

Physical Properties

Property code	Value	Unit	Source
gf	-105.23	kJ/mol	Joback Method
hf	-466.98	kJ/mol	Joback Method
hfus	28.61	kJ/mol	Joback Method
hvap	55.28	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.949		Crippen Method
mcvol	183.270	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1486.00		NIST Webbook
tb	577.10	K	Joback Method
tc	753.70	K	Joback Method
tf	323.55	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.14	J/mol×K	577.10	Joback Method
cpg	485.47	J/mol×K	606.53	Joback Method
cpg	500.16	J/mol×K	635.97	Joback Method
cpg	514.20	J/mol×K	665.40	Joback Method
cpg	527.61	J/mol×K	694.84	Joback Method
cpg	540.39	J/mol×K	724.27	Joback Method
cpg	552.57	J/mol×K	753.70	Joback Method

Sources

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=R392602&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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