Isobutylcarbamate, N,N-dihexyl

Inchi: InChI=1S/C17H35NO2/c1-5-7-9-11-13-18(14-12-10-8-6-2)17(19)20-15-16(3)4/h16H,5-15
InchiKey: XPZRRQRGZPQIPJ-UHFFFAOYSA-N
Formula: C17H35NO2
SMILES: CCCCCCN(CCCCCC)C(=O)OCC(C)C
Mol. weight [g/mol]: 285.47

Physical Properties

Property code	Value	Unit	Source
gf	-33.32	kJ/mol	Joback Method
hf	-576.76	kJ/mol	Joback Method
hfus	42.07	kJ/mol	Joback Method
hvap	64.25	kJ/mol	Joback Method
log10ws	-5.11		Crippen Method
logp	5.242		Crippen Method
mcvol	267.810	ml/mol	McGowan Method
pc	1277.33	kPa	Joback Method
rinpol	1863.00		NIST Webbook
tb	676.65	K	Joback Method
tc	845.94	K	Joback Method
tf	370.98	K	Joback Method
vc	1.024	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.15	J/mol×K	676.65	Joback Method
cpg	792.97	J/mol×K	704.86	Joback Method
cpg	810.93	J/mol×K	733.08	Joback Method
cpg	828.05	J/mol×K	761.29	Joback Method
cpg	844.35	J/mol×K	789.51	Joback Method
cpg	859.86	J/mol×K	817.72	Joback Method
cpg	874.60	J/mol×K	845.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392662&Units=SI
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

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