Isobutylcarbamate, N-pentyl

Inchi: InChI=1S/C15H31NO2/c1-5-7-9-11-16(12-10-8-6-2)15(17)18-13-14(3)4/h14H,5-13H2,1-4
InchiKey: XMENVGIGUYLHTP-UHFFFAOYSA-N
Formula: C15H31NO2
SMILES: CCCCCN(CCCCC)C(=O)OCC(C)C
Mol. weight [g/mol]: 257.41

Physical Properties

Property code	Value	Unit	Source
gf	-50.16	kJ/mol	Joback Method
hf	-535.48	kJ/mol	Joback Method
hfus	36.89	kJ/mol	Joback Method
hvap	59.80	kJ/mol	Joback Method
log10ws	-4.27		Crippen Method
logp	4.461		Crippen Method
mcvol	239.630	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
rinpol	1380.00		NIST Webbook
rinpol	1380.00		NIST Webbook
tb	630.89	K	Joback Method
tc	800.00	K	Joback Method
tf	348.44	K	Joback Method
vc	0.911	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	661.02	J/mol×K	630.89	Joback Method
cpg	679.02	J/mol×K	659.07	Joback Method
cpg	696.23	J/mol×K	687.26	Joback Method
cpg	712.66	J/mol×K	715.44	Joback Method
cpg	728.33	J/mol×K	743.63	Joback Method
cpg	743.26	J/mol×K	771.81	Joback Method
cpg	757.47	J/mol×K	800.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392711&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