Isobutylcarbamate, N-decyl

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

Physical Properties

Property code	Value	Unit	Source
gf	-71.55	kJ/mol	Joback Method
hf	-549.54	kJ/mol	Joback Method
hfus	38.97	kJ/mol	Joback Method
hvap	64.19	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.509		Crippen Method
mcvol	239.630	ml/mol	McGowan Method
pc	1489.58	kPa	Joback Method
rinpol	1881.00		NIST Webbook
tb	668.62	K	Joback Method
tc	841.93	K	Joback Method
tf	368.63	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.08	J/mol×K	668.62	Joback Method
cpg	700.49	J/mol×K	697.50	Joback Method
cpg	717.11	J/mol×K	726.39	Joback Method
cpg	732.95	J/mol×K	755.27	Joback Method
cpg	748.02	J/mol×K	784.16	Joback Method
cpg	762.34	J/mol×K	813.04	Joback Method
cpg	775.94	J/mol×K	841.93	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=R392573&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