Isobutylcarbamate, N,Np-diisobutyl

Inchi: InChI=1S/C13H27NO2/c1-10(2)7-14(8-11(3)4)13(15)16-9-12(5)6/h10-12H,7-9H2,1-6H3
InchiKey: XZROWWVBAKDDEX-UHFFFAOYSA-N
Formula: C13H27NO2
SMILES: CC(C)COC(=O)N(CC(C)C)CC(C)C
Mol. weight [g/mol]: 229.36

Physical Properties

Property code	Value	Unit	Source
gf	-71.88	kJ/mol	Joback Method
hf	-504.76	kJ/mol	Joback Method
hfus	24.66	kJ/mol	Joback Method
hvap	54.57	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	3.393		Crippen Method
mcvol	211.450	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	1399.00		NIST Webbook
tb	584.25	K	Joback Method
tc	760.47	K	Joback Method
tf	295.90	K	Joback Method
vc	0.787	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.81	J/mol×K	584.25	Joback Method
cpg	571.55	J/mol×K	613.62	Joback Method
cpg	588.49	J/mol×K	642.99	Joback Method
cpg	604.65	J/mol×K	672.36	Joback Method
cpg	620.05	J/mol×K	701.73	Joback Method
cpg	634.70	J/mol×K	731.10	Joback Method
cpg	648.62	J/mol×K	760.47	Joback Method

Sources

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=R392697&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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