Isobutylcarbamate, N,N-diisopropyl

Inchi: InChI=1S/C11H23NO2/c1-8(2)7-14-11(13)12(9(3)4)10(5)6/h8-10H,7H2,1-6H3
InchiKey: FLHIACVLZLMEPA-UHFFFAOYSA-N
Formula: C11H23NO2
SMILES: CC(C)COC(=O)N(C(C)C)C(C)C
Mol. weight [g/mol]: 201.31

Physical Properties

Property code	Value	Unit	Source
gf	-88.72	kJ/mol	Joback Method
hf	-463.48	kJ/mol	Joback Method
hfus	19.48	kJ/mol	Joback Method
hvap	50.12	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.898		Crippen Method
mcvol	183.270	ml/mol	McGowan Method
pc	2054.89	kPa	Joback Method
rinpol	1252.00		NIST Webbook
tb	538.49	K	Joback Method
tc	717.80	K	Joback Method
tf	273.36	K	Joback Method
vc	0.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.87	J/mol×K	538.49	Joback Method
cpg	468.48	J/mol×K	568.38	Joback Method
cpg	484.37	J/mol×K	598.26	Joback Method
cpg	499.53	J/mol×K	628.15	Joback Method
cpg	513.99	J/mol×K	658.03	Joback Method
cpg	527.76	J/mol×K	687.92	Joback Method
cpg	540.85	J/mol×K	717.80	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392677&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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