Isobutylcarbamate, N-butyl

Inchi: InChI=1S/C9H19NO2/c1-4-5-6-10-9(11)12-7-8(2)3/h8H,4-7H2,1-3H3,(H,10,11)
InchiKey: LNQSASGEEAOEOM-UHFFFAOYSA-N
Formula: C9H19NO2
SMILES: CCCCNC(=O)OCC(C)C
Mol. weight [g/mol]: 173.25

Physical Properties

Property code	Value	Unit	Source
gf	-122.07	kJ/mol	Joback Method
hf	-425.70	kJ/mol	Joback Method
hfus	23.43	kJ/mol	Joback Method
hvap	50.83	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.169		Crippen Method
mcvol	155.090	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1282.00		NIST Webbook
tb	531.34	K	Joback Method
tc	711.14	K	Joback Method
tf	301.01	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.98	J/mol×K	531.34	Joback Method
cpg	386.87	J/mol×K	561.31	Joback Method
cpg	400.20	J/mol×K	591.27	Joback Method
cpg	412.96	J/mol×K	621.24	Joback Method
cpg	425.16	J/mol×K	651.21	Joback Method
cpg	436.82	J/mol×K	681.18	Joback Method
cpg	447.93	J/mol×K	711.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392553&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