Isobutylcarbamate, N,N-diethyl

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

Physical Properties

Property code	Value	Unit	Source
gf	-100.68	kJ/mol	Joback Method
hf	-411.64	kJ/mol	Joback Method
hfus	21.35	kJ/mol	Joback Method
hvap	46.44	kJ/mol	Joback Method
log10ws	-1.76		Crippen Method
logp	2.121		Crippen Method
mcvol	155.090	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	1162.00		NIST Webbook
tb	493.61	K	Joback Method
tc	669.14	K	Joback Method
tf	280.82	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.39	J/mol×K	493.61	Joback Method
cpg	370.77	J/mol×K	522.87	Joback Method
cpg	384.56	J/mol×K	552.12	Joback Method
cpg	397.78	J/mol×K	581.38	Joback Method
cpg	410.42	J/mol×K	610.63	Joback Method
cpg	422.51	J/mol×K	639.89	Joback Method
cpg	434.06	J/mol×K	669.14	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=R392657&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