Isobutylcarbamate, N-ethyl-N-methyl

Inchi: InChI=1S/C8H17NO2/c1-5-9(4)8(10)11-6-7(2)3/h7H,5-6H2,1-4H3
InchiKey: JEEZBDJTOQTVPP-UHFFFAOYSA-N
Formula: C8H17NO2
SMILES: CCN(C)C(=O)OCC(C)C
Mol. weight [g/mol]: 159.23

Physical Properties

Property code	Value	Unit	Source
gf	-109.10	kJ/mol	Joback Method
hf	-391.00	kJ/mol	Joback Method
hfus	18.76	kJ/mol	Joback Method
hvap	44.21	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	1.731		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
rinpol	1101.00		NIST Webbook
rinpol	1101.00		NIST Webbook
tb	470.73	K	Joback Method
tc	647.78	K	Joback Method
tf	269.55	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	311.72	J/mol×K	470.73	Joback Method
cpg	325.21	J/mol×K	500.24	Joback Method
cpg	338.14	J/mol×K	529.75	Joback Method
cpg	350.55	J/mol×K	559.25	Joback Method
cpg	362.43	J/mol×K	588.76	Joback Method
cpg	373.79	J/mol×K	618.27	Joback Method
cpg	384.64	J/mol×K	647.78	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=R392588&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