Isobutylcarbamate, N-cyclohexyl

Inchi: InChI=1S/C11H21NO2/c1-9(2)8-14-11(13)12-10-6-4-3-5-7-10/h9-10H,3-8H2,1-2H3,(H,12
InchiKey: FCYDEXVOKLZLPO-UHFFFAOYSA-N
Formula: C11H21NO2
SMILES: CC(C)COC(=O)NC1CCCCC1
Mol. weight [g/mol]: 199.29

Physical Properties

Property code	Value	Unit	Source
gf	-80.78	kJ/mol	Joback Method
hf	-412.66	kJ/mol	Joback Method
hfus	20.44	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Joback Method
log10ws	-3.22		Crippen Method
logp	2.701		Crippen Method
mcvol	172.410	ml/mol	McGowan Method
pc	2495.01	kPa	Joback Method
rinpol	1515.00		NIST Webbook
rinpol	1515.00		NIST Webbook
tb	596.65	K	Joback Method
tc	803.51	K	Joback Method
tf	330.93	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	460.83	J/mol×K	596.65	Joback Method
cpg	479.38	J/mol×K	631.13	Joback Method
cpg	496.89	J/mol×K	665.60	Joback Method
cpg	513.39	J/mol×K	700.08	Joback Method
cpg	528.89	J/mol×K	734.56	Joback Method
cpg	543.41	J/mol×K	769.04	Joback Method
cpg	556.97	J/mol×K	803.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392568&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