Isobutylcarbamate, N,N-dicyclohexyl

Inchi: InChI=1S/C17H31NO2/c1-14(2)13-20-17(19)18(15-9-5-3-6-10-15)16-11-7-4-8-12-16/h14
InchiKey: UHHDLFPECWRPPD-UHFFFAOYSA-N
Formula: C17H31NO2
SMILES: CC(C)COC(=O)N(C1CCCCC1)C1CCCCC1
Mol. weight [g/mol]: 281.43

Physical Properties

Property code	Value	Unit	Source
gf	15.58	kJ/mol	Joback Method
hf	-468.12	kJ/mol	Joback Method
hfus	25.74	kJ/mol	Joback Method
hvap	65.11	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.746		Crippen Method
mcvol	246.090	ml/mol	McGowan Method
pc	1753.60	kPa	Joback Method
rinpol	1973.00		NIST Webbook
rinpol	1973.00		NIST Webbook
tb	715.75	K	Joback Method
tc	933.03	K	Joback Method
tf	385.74	K	Joback Method
vc	0.889	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	767.59	J/mol×K	715.75	Joback Method
cpg	791.43	J/mol×K	751.96	Joback Method
cpg	813.59	J/mol×K	788.18	Joback Method
cpg	834.15	J/mol×K	824.39	Joback Method
cpg	853.14	J/mol×K	860.61	Joback Method
cpg	870.62	J/mol×K	896.82	Joback Method
cpg	886.64	J/mol×K	933.03	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392642&Units=SI

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