Isobutylcarbamate, N,N-dibutyl

Inchi: InChI=1S/C13H27NO2/c1-5-7-9-14(10-8-6-2)13(15)16-11-12(3)4/h12H,5-11H2,1-4H3
InchiKey: BAGZNMSPKRGKFK-UHFFFAOYSA-N
Formula: C13H27NO2
SMILES: CCCCN(CCCC)C(=O)OCC(C)C
Mol. weight [g/mol]: 229.36

Physical Properties

Property code	Value	Unit	Source
gf	-67.00	kJ/mol	Joback Method
hf	-494.20	kJ/mol	Joback Method
hfus	31.71	kJ/mol	Joback Method
hvap	55.34	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	3.681		Crippen Method
mcvol	211.450	ml/mol	McGowan Method
pc	1716.03	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	585.13	K	Joback Method
tc	755.50	K	Joback Method
tf	325.90	K	Joback Method
vc	0.799	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.18	J/mol×K	585.13	Joback Method
cpg	570.23	J/mol×K	613.52	Joback Method
cpg	586.55	J/mol×K	641.92	Joback Method
cpg	602.16	J/mol×K	670.31	Joback Method
cpg	617.06	J/mol×K	698.71	Joback Method
cpg	631.27	J/mol×K	727.10	Joback Method
cpg	644.82	J/mol×K	755.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R392637&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

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