Isobutylcarbamate, N-tert.-butyl

Inchi: InChI=1S/C13H27NO2/c1-10(2)9-16-11(15)14(12(3,4)5)13(6,7)8/h10H,9H2,1-8H3
InchiKey: ITYARLOMXDAOCM-UHFFFAOYSA-N
Formula: C13H27NO2
SMILES: CC(C)COC(=O)N(C(C)(C)C)C(C)(C)C
Mol. weight [g/mol]: 229.36

Physical Properties

Property code	Value	Unit	Source
gf	-61.32	kJ/mol	Joback Method
hf	-511.70	kJ/mol	Joback Method
hfus	16.88	kJ/mol	Joback Method
hvap	52.75	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.678		Crippen Method
mcvol	211.450	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1121.00		NIST Webbook
tb	578.67	K	Joback Method
tc	766.80	K	Joback Method
tf	330.74	K	Joback Method
vc	0.777	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	558.70	J/mol×K	578.67	Joback Method
cpg	577.54	J/mol×K	610.02	Joback Method
cpg	595.32	J/mol×K	641.38	Joback Method
cpg	612.10	J/mol×K	672.73	Joback Method
cpg	627.92	J/mol×K	704.09	Joback Method
cpg	642.83	J/mol×K	735.44	Joback Method
cpg	656.87	J/mol×K	766.80	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=R392731&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