Isobutylcarbamate, N-isopentyl

Inchi: InChI=1S/C10H21NO2/c1-8(2)5-6-11-10(12)13-7-9(3)4/h8-9H,5-7H2,1-4H3,(H,11,12)
InchiKey: YKOGCEHPFADOFB-UHFFFAOYSA-N
Formula: C10H21NO2
SMILES: CC(C)CCNC(=O)OCC(C)C
Mol. weight [g/mol]: 187.28

Physical Properties

Property code	Value	Unit	Source
gf	-116.09	kJ/mol	Joback Method
hf	-451.62	kJ/mol	Joback Method
hfus	22.50	kJ/mol	Joback Method
hvap	52.67	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.415		Crippen Method
mcvol	169.180	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
rinpol	1345.00		NIST Webbook
tb	553.78	K	Joback Method
tc	735.28	K	Joback Method
tf	297.28	K	Joback Method
vc	0.642	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.01	J/mol×K	553.78	Joback Method
cpg	436.00	J/mol×K	584.03	Joback Method
cpg	450.35	J/mol×K	614.28	Joback Method
cpg	464.07	J/mol×K	644.53	Joback Method
cpg	477.16	J/mol×K	674.78	Joback Method
cpg	489.63	J/mol×K	705.03	Joback Method
cpg	501.50	J/mol×K	735.28	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=R392622&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