

Isobutylcarbamate, N,N-dipropyl

Inchi:	InChI=1S/C11H23NO2/c1-5-7-12(8-6-2)11(13)14-9-10(3)4/h10H,5-9H2,1-4H3
InchiKey:	GXJCJFIMKNFAQG-UHFFFAOYSA-N
Formula:	C11H23NO2
SMILES:	CCCN(CCC)C(=O)OCC(C)C
Mol. weight [g/mol]:	201.31

Physical Properties

Property code	Value	Unit	Source
gf	-83.84	kJ/mol	Joback Method
hf	-452.92	kJ/mol	Joback Method
hfus	26.53	kJ/mol	Joback Method
hvap	50.89	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.901		Crippen Method
mvol	183.270	ml/mol	McGowan Method
pc	2025.41	kPa	Joback Method
rinsol	1323.00		NIST Webbook
tb	539.37	K	Joback Method
tc	712.03	K	Joback Method
tf	303.36	K	Joback Method
vc	0.688	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.37	J/mol×K	539.37	Joback Method
cpg	467.25	J/mol×K	568.15	Joback Method
cpg	482.46	J/mol×K	596.92	Joback Method
cpg	497.02	J/mol×K	625.70	Joback Method
cpg	510.94	J/mol×K	654.47	Joback Method
cpg	524.23	J/mol×K	683.25	Joback Method
cpg	536.91	J/mol×K	712.03	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R392682&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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