

N-Isobutylformamide

Other names:	Formamide, N-isobutyl-
Inchi:	InChI=1S/C5H11NO/c1-5(2)3-6-4-7/h4-5H,3H2,1-2H3,(H,6,7)
InchiKey:	XCTTVNSXEHWZBI-UHFFFAOYSA-N
Formula:	C5H11NO
SMILES:	CC(C)CN=CO
Mol. weight [g/mol]:	101.15
CAS:	6281-96-5

Physical Properties

Property code	Value	Unit	Source
hf	-221.82	kJ/mol	Joback Method
hvap	46.33	kJ/mol	Joback Method
log10ws	-0.66		Crippen Method
logp	1.229		Crippen Method
mcvol	92.860	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1014.00		NIST Webbook
rinpol	1014.00		NIST Webbook
ripol	1759.00		NIST Webbook
ripol	1759.00		NIST Webbook
tb	482.22	K	Joback Method
tc	667.10	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6281965&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

hf:	Enthalpy of formation 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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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