

Formamidine, 1-isobutyl-3,3-hexamethyleno

Inchi:	InChI=1S/C11H22N2/c1-11(2)9-12-10-13-7-5-3-4-6-8-13/h10-11H,3-9H2,1-2H3/b12-10+
InchiKey:	IECMLFDQMAHNRP-ZRDIBKRKSA-N
Formula:	C11H22N2
SMILES:	CC(C)CN=CN1CCCCC1
Mol. weight [g/mol]:	182.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	2.547		Crippen Method
mcvol	170.650	ml/mol	McGowan Method
rinpola	1423.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R118395&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices

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