

Formamidine, 3,3-hexamethyleno-1-propyl

Inchi:	InChI=1S/C10H20N2/c1-2-7-11-10-12-8-5-3-4-6-9-12/h10H,2-9H2,1H3/b11-10+
InchiKey:	BIEGWMCNZNNTHD-ZHACJKMWSA-N
Formula:	C10H20N2
SMILES:	CCCN=CN1CCCCC1
Mol. weight [g/mol]:	168.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	2.301		Crippen Method
mcvol	156.560	ml/mol	McGowan Method
rinpol	1378.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R118706&Units=SI

Legend

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

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