

4-Hexamethyleneiminobutyronitrile

Other names:	4-(n-Hexamethyleneimino)butyronitrile 1H-Azepine-1-butanenitrile, hexahydro- Butyronitrile, 1-(hexahydro-1H-azepin-1-yl)- 1H-Azepine-1-butyronitrile, hexahydro- 1-(Hexahydro-1H-azepin-1-yl)butyronitrile hexahydro-1H-azepine-1-butyronitrile
Inchi:	InChI=1S/C10H18N2/c11-7-3-6-10-12-8-4-1-2-5-9-12/h1-6,8-10H2
InchiKey:	OQPSAQBHEQYYMJ-UHFFFAOYSA-N
Formula:	C10H18N2
SMILES:	N#CCCCN1CCCCC1
Mol. weight [g/mol]:	166.26
CAS:	3194-43-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	2.166		Crippen Method
mcvol	152.260	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3194432&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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