

Hexamethyleneiminoacetonitrile

Other names: 2-(n-Hexamethyleneimino)acetonitrile
(n-Hexamethyleneimino)acetonitrile
1H-Azepine-1-acetonitrile, hexahydro-
Acetonitrile, (hexahydro-1H-azepin-1-yl)-
Hexahydro-1H-azepine-1-acetonitrile

Inchi: InChI=1S/C8H14N2/c9-5-8-10-6-3-1-2-4-7-10/h1-4,6-8H2

InchiKey: OHKGIEVCPHMZKY-UHFFFAOYSA-N

Formula: C8H14N2

SMILES: N#CCN1CCCCC1

Mol. weight [g/mol]: 138.21

CAS: 54714-50-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.50		Crippen Method
logp	1.386		Crippen Method
mcvol	124.080	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C54714500&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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<https://www.chemeo.com/cid/39-911-7/Hexamethyleneiminoacetonitrile.pdf>

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