

N-Ethyl-hexahydro-1H-azepine

Other names:	1-Ethyl-hexahydroazepine
Inchi:	InChI=1S/C8H17N/c1-2-9-7-5-3-4-6-8-9/h2-8H2,1H3
InchiKey:	RUOFIIKCANAEBW-UHFFFAOYSA-N
Formula:	C8H17N
SMILES:	CCN1CCCCC1
Mol. weight [g/mol]:	127.23
CAS:	6763-91-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.64		Crippen Method
logp	1.882		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
rinsol	954.00		NIST Webbook
rinsol	954.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6763913&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
rinsol:	Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/35-730-2/N-Ethyl-hexahydro-1H-azepine.pdf>

Generated by Cheméo on 2024-04-29 04:38:57.121946846 +0000 UTC m=+16654786.042524165.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.