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: CCN1CCCCCC1
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
rinpol	954.00		NIST Webbook
rinpol	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/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
rinpol: Non-polar retention indices

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