Pyrrolidine, 1-ethyl-

Other names: N-ethyl-Tetrahydropyrrole
1-Ethyl-pyrrolidine
Inchi: InChI=1S/C6H13N/c1-2-7-5-3-4-6-7/h2-6H2,1H3
InchiKey: ONQBOTKLCMXPOF-UHFFFAOYSA-N
Formula: C6H13N
SMILES: CCN1CCCC1
Mol. weight [g/mol]: 99.17
CAS: 7335-06-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.80		Crippen Method
logp	1.102		Crippen Method
mcvol	94.520	ml/mol	McGowan Method
rinpol	751.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	761.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	751.00		NIST Webbook
rinpol	750.00		NIST Webbook
rinpol	753.00		NIST Webbook
rinpol	774.00		NIST Webbook
ripol	930.00		NIST Webbook
ripol	930.00		NIST Webbook
ripol	906.00		NIST Webbook

Sources

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=C7335060&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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