

N-(2-mercaptoethyl)pyrrole

Inchi: InChI=1S/C6H9NS/c8-6-5-7-3-1-2-4-7/h1-4,8H,5-6H2
InchiKey: LARJPSNKEASDID-UHFFFAOYSA-N
Formula: C6H9NS
SMILES: SCCn1cccc1
Mol. weight [g/mol]: 127.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.80		Crippen Method
logp	1.418		Crippen Method
mcvol	102.270	ml/mol	McGowan Method
rinpol	1110.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1755.00		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=R239299&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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<https://www.cheméo.com/cid/32-853-9/N-2-mercaptoethyl-pyrrole.pdf>

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