

1H-Pyrrole, 1-methyl-2-propyl

Inchi: InChI=1S/C8H13N/c1-3-5-8-6-4-7-9(8)2/h4,6-7H,3,5H2,1-2H3
InchiKey: REFXEKIEYCQSQN-UHFFFAOYSA-N
Formula: C8H13N
SMILES: CCCc1cccn1C
Mol. weight [g/mol]: 123.20

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.98		Crippen Method
logp	1.978		Crippen Method
mcvol	114.100	ml/mol	McGowan Method
rinpol	1056.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1056.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R62976&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
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
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/28-175-7/1H-Pyrrole-1-methyl-2-propyl.pdf>

Generated by Cheméo on 2024-04-19 18:47:16.778620645 +0000 UTC m=+15841685.699197960.
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.