

1-(3-Methylbutyl)pyrrole

Inchi: InChI=1S/C9H15N/c1-9(2)5-8-10-6-3-4-7-10/h3-4,6-7,9H,5,8H2,1-2H3
InchiKey: QNFYLUDDPMZVIOU-UHFFFAOYSA-N
Formula: C9H15N
SMILES: CC(C)CCn1cccc1
Mol. weight [g/mol]: 137.22

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.75		Crippen Method
logp	2.534		Crippen Method
mcvol	128.190	ml/mol	McGowan Method
ripol	1378.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1378.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R547590&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.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
ripol: Polar retention indices

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