

1H-Imidazole, 4-methyl-1-propyl

Inchi: InChI=1S/C7H12N2/c1-3-4-9-5-7(2)8-6-9/h5-6H,3-4H2,1-2H3
InchiKey: SCHMIVXQOZZUFW-UHFFFAOYSA-N
Formula: C7H12N2
SMILES: CCCn1cnc(C)c1
Mol. weight [g/mol]: 124.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.39		Crippen Method
logp	1.602		Crippen Method
mcvol	109.990	ml/mol	McGowan Method
rinpol	1120.00		NIST Webbook
rinpol	1120.00		NIST Webbook
ripol	1766.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R68370&Units=SI>

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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