1H-Imidazole, 4-methyl-1-pentyl

Inchi: InChI=1S/C9H16N2/c1-3-4-5-6-11-7-9(2)10-8-11/h7-8H,3-6H2,1-2H3
InchiKey: XKFFEMCWONYMOP-UHFFFAOYSA-N
Formula: C9H16N2
SMILES: CCCCCn1cnc(C)c1
Mol. weight [g/mol]: 152.24

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	2.382		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
rinpol	1313.00		NIST Webbook
ripol	1954.00		NIST Webbook
ripol	1954.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R68366&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol: Polar retention indices

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