

1H-Imidazole, 1-ethyl-4-methyl

Inchi: InChI=1S/C6H10N2/c1-3-8-4-6(2)7-5-8/h4-5H,3H2,1-2H3
InchiKey: JXZUHDMMANYKMX-UHFFFAOYSA-N
Formula: C6H10N2
SMILES: CCn1cnc(C)c1
Mol. weight [g/mol]: 110.16

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.97		Crippen Method
logp	1.211		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
rinpol	1044.00		NIST Webbook
rinpol	1044.00		NIST Webbook
ripol	1712.00		NIST Webbook
ripol	1712.00		NIST Webbook

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R68316&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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