

4-Methylpyridazine

Inchi: InChI=1S/C5H6N2/c1-5-2-3-6-7-4-5/h2-4H,1H3
InchiKey: AIKUBOPKWKZULG-UHFFFAOYSA-N
Formula: C5H6N2
SMILES: Cc1ccnnc1
Mol. weight [g/mol]: 94.11
CAS: 1120-88-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.48		Crippen Method
logp	0.785		Crippen Method
mcvol	77.510	ml/mol	McGowan Method
rinpola	1045.00		NIST Webbook
rinpola	1045.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1120883&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
rinpola: Non-polar retention indices

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<https://www.chemeo.com/cid/80-824-8/4-Methylpyridazine.pdf>

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