

4-Methylpyrrolo[1,2-a]pyrazine

Other names: 4-Methylpyrrol-1,2-A-pyrazine
Inchi: InChI=1S/C8H8N2/c1-7-5-9-6-8-3-2-4-10(7)8/h2-6H,1H3
InchiKey: GCXGRZISVBCADH-UHFFFAOYSA-N
Formula: C8H8N2
SMILES: Cc1cncc2cccn12
Mol. weight [g/mol]: 132.16
CAS: 64608-60-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.67		Crippen Method
logp	1.643		Crippen Method
mcvol	104.620	ml/mol	McGowan Method
rinpol	1340.00		NIST Webbook
rinpol	1340.00		NIST Webbook
ripol	2093.00		NIST Webbook
ripol	2167.00		NIST Webbook

Sources

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=C64608602&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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