

Pyrazine, 2-methyl-5-methylthio

Other names: 5-Methyl-2-(methylthio)pyrazine
Inchi: InChI=1S/C6H8N2S/c1-5-3-8-6(9-2)4-7-5/h3-4H,1-2H3
InchiKey: DNBQBSWEJGAAIY-UHFFFAOYSA-N
Formula: C6H8N2S
SMILES: CSc1cnc(C)cn1
Mol. weight [g/mol]: 140.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.22		Crippen Method
logp	1.507		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
rinpol	1163.00		NIST Webbook
rinpol	1166.00		NIST Webbook
rinpol	1166.00		NIST Webbook
ripol	1678.00		NIST Webbook
ripol	1678.00		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=R38676&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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