

5-Isobutyl-3-methyl-2-(methylthio)pyrazine

Other names: Pyrazine, 3-methyl-5-(2-methylpropyl)-2-(methylthio)
Inchi: InChI=1S/C10H16N2S/c1-7(2)5-9-6-11-10(13-4)8(3)12-9/h6-7H,5H2,1-4H3
InchiKey: OYANNTFZVSVJHE-UHFFFAOYSA-N
Formula: C10H16N2S
SMILES: CSc1ncc(CC(C)C)nc1C
Mol. weight [g/mol]: 196.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	2.705		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
rinpol	1446.00		NIST Webbook
rinpol	1446.00		NIST Webbook
ripol	1816.00		NIST Webbook
ripol	1816.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R38608&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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