

2-Ethylthio-5-isopropyl-3-methylpyrazine

Other names: Pyrazine, 2-(ethylthio)-3-methyl-5-(1-methylethyl)
Inchi: InChI=1S/C10H16N2S/c1-5-13-10-8(4)12-9(6-11-10)7(2)3/h6-7H,5H2,1-4H3
InchiKey: JWTDEQFQCSRVIV-UHFFFAOYSA-N
Formula: C10H16N2S
SMILES: CCSc1ncc(C(C)C)nc1C
Mol. weight [g/mol]: 196.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.83		Crippen Method
logp	3.020		Crippen Method
mcvol	164.310	ml/mol	McGowan Method
rinpol	1418.00		NIST Webbook
rinpol	1418.00		NIST Webbook
ripol	1769.00		NIST Webbook
ripol	1769.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R38402&Units=SI>
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>

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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