

Pyrazine, 2-(ethylthio)-3-methyl-5-(2-methylpropyl)

Other names: 2-Ethylthio-5-isobutyl-3-methylpyrazine
Inchi: InChI=1S/C11H18N2S/c1-5-14-11-9(4)13-10(7-12-11)6-8(2)3/h7-8H,5-6H2,1-4H3
InchiKey: YRNUTGLMZZOETN-UHFFFAOYSA-N
Formula: C11H18N2S
SMILES: CCSc1ncc(CC(C)C)nc1C
Mol. weight [g/mol]: 210.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	3.096		Crippen Method
mcvol	178.400	ml/mol	McGowan Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
ripol	1843.00		NIST Webbook
ripol	1843.00		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=R38395&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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