

2-ethylthio-3-methyl-5-(2-methylbutyl)pyrazine

Other names: Pyrazine, 2-(ethylthio)-3-methyl-5-(2-methylbutyl)
Inchi: InChI=1S/C12H20N2S/c1-5-9(3)7-11-8-13-12(15-6-2)10(4)14-11/h8-9H,5-7H2,1-4H3
InchiKey: NSUWJTNHTHHKPF-UHFFFAOYSA-N
Formula: C12H20N2S
SMILES: CCSc1ncc(CC(C)CC)nc1C
Mol. weight [g/mol]: 224.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.46		Crippen Method
logp	3.486		Crippen Method
mcvol	192.490	ml/mol	McGowan Method
rinpol	1602.00		NIST Webbook
ripol	1951.00		NIST Webbook
ripol	1951.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
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=R38363&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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