

Pyrazine, 2-(methylthio)-3-octyl

Other names: Pyrazine, 3-methylthio-2-octyl
Inchi: InChI=1S/C13H22N2S/c1-3-4-5-6-7-8-9-12-13(16-2)15-11-10-14-12/h10-11H,3-9H2,1-2H
InchiKey: WRMWXTXUDAAVIW-UHFFFAOYSA-N
Formula: C13H22N2S
SMILES: CCCCCCCc1nccnc1SC
Mol. weight [g/mol]: 238.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	4.101		Crippen Method
mcvol	206.580	ml/mol	McGowan Method
rinpol	1825.00		NIST Webbook
rinpol	1825.00		NIST Webbook
ripol	2287.00		NIST Webbook
ripol	2287.00		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=R43766&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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