

Pyrazine, 2-methoxy-3-octyl

Other names: Pyrazine, 3-methoxy-2-octyl
Inchi: InChI=1S/C13H22N2O/c1-3-4-5-6-7-8-9-12-13(16-2)15-11-10-14-12/h10-11H,3-9H2,1-2H
InchiKey: YZEKUSSOIBZUIS-UHFFFAOYSA-N
Formula: C13H22N2O
SMILES: CCCCCCCCc1nccnc1OC
Mol. weight [g/mol]: 222.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.44		Crippen Method
logp	3.388		Crippen Method
mcvol	196.100	ml/mol	McGowan Method
rinpol	1613.00		NIST Webbook
rinpol	1613.00		NIST Webbook
ripol	1966.00		NIST Webbook
ripol	1966.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R43748&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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