

Pyrazine, 2-isoheptyl-3-methoxy

Other names: Pyrazine, 2-(4-methylpentyl)-3-methoxy
Inchi: InChI=1S/C11H18N2O/c1-9(2)5-4-6-10-11(14-3)13-8-7-12-10/h7-9H,4-6H2,1-3H3
InchiKey: HQNJHPJFKOLFHC-UHFFFAOYSA-N
Formula: C11H18N2O
SMILES: COc1nccnc1CCCC(C)C
Mol. weight [g/mol]: 194.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	2.464		Crippen Method
mcvol	167.920	ml/mol	McGowan Method
rinpol	1388.00		NIST Webbook
rinpol	1388.00		NIST Webbook
ripol	1711.00		NIST Webbook
ripol	1711.00		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=R43378&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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