

Pyrazine, 2-heptyl-3-methoxy

Inchi: InChI=1S/C12H20N2O/c1-3-4-5-6-7-8-11-12(15-2)14-10-9-13-11/h9-10H,3-8H2,1-2H3
InchiKey: PPSICHXRNPVJZ-UHFFFAOYSA-N
Formula: C12H20N2O
SMILES: CCCCCCc1nccnc1OC
Mol. weight [g/mol]: 208.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.02		Crippen Method
logp	2.998		Crippen Method
mcvol	182.010	ml/mol	McGowan Method
rinpol	1519.00		NIST Webbook
rinpol	1519.00		NIST Webbook
ripol	1867.00		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=R43449&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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