

Pyrazine, 2-methoxy-3-propyl

Inchi: InChI=1S/C8H12N2O/c1-3-4-7-8(11-2)10-6-5-9-7/h5-6H,3-4H2,1-2H3
InchiKey: WPWBOFKCKQCZIS-UHFFFAOYSA-N
Formula: C8H12N2O
SMILES: CCCc1nccnc1OC
Mol. weight [g/mol]: 152.19

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.34		Crippen Method
logp	1.438		Crippen Method
mcvol	125.650	ml/mol	McGowan Method
rinpol	1121.00		NIST Webbook
ripol	1470.00		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=R43499&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

Latest version available from:

<https://www.chemeo.com/cid/29-498-8/Pyrazine-2-methoxy-3-propyl.pdf>

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