

2-methoxy-3,5-dimethylpyrazine

Inchi: InChI=1S/C7H10N2O/c1-5-4-8-7(10-3)6(2)9-5/h4H,1-3H3
InchiKey: BXKLSVWRSUPMBO-UHFFFAOYSA-N
Formula: C7H10N2O
SMILES: COc1ncc(C)nc1C
Mol. weight [g/mol]: 138.17

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.07		Crippen Method
logp	1.102		Crippen Method
mcpvol	111.560	ml/mol	McGowan Method
ripol	1054.00		NIST Webbook
ripol	1055.00		NIST Webbook
ripol	1040.00		NIST Webbook
ripol	1423.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1433.00		NIST Webbook
ripol	1450.00		NIST Webbook
ripol	1423.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R234670&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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