

3-Methoxy-5-methylpyrazine 1-Oxide

Inchi: InChI=1S/C6H8N2O2/c1-5-3-8(9)4-6(7-5)10-2/h3-4H,1-2H3
InchiKey: JPKZYYICYSAJPM-UHFFFAOYSA-N
Formula: C6H8N2O2
SMILES: COc1c[n+](O-)cc(C)n1
Mol. weight [g/mol]: 140.14

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.36		Crippen Method
logp	0.032		Crippen Method
mcvol	103.340	ml/mol	McGowan Method
rinpol	1375.00		NIST Webbook
rinpol	1375.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R412865&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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