

Pyrazine, 2,5-dimethyl-, 1,4-dioxide

Other names:	2,5-dimethylpyrazine 1,4-dioxide
Inchi:	InChI=1S/C6H8N2O2/c1-5-3-8(10)6(2)4-7(5)9/h3-4H,1-2H3
InchiKey:	QQWHPPCKIBOLLX-UHFFFAOYSA-N
Formula:	C6H8N2O2
SMILES:	Cc1c[n+](O)c(C)c[n+]1O
Mol. weight [g/mol]:	140.14
CAS:	6890-38-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	-0.430		Crippen Method
mcvol	103.340	ml/mol	McGowan Method

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=C6890386&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

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<https://www.chemeo.com/cid/124-537-8/Pyrazine-2-5-dimethyl-1-4-dioxide.pdf>

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