

Pyrazine, 2-acetyl-3,6-dimethyl

Other names:	2-Acetyl-3,6-dimethylpyrazine 1-(3,6-dimethylpyrazinyl)ethan-1-one
Inchi:	InChI=1S/C8H10N2O/c1-5-4-9-6(2)8(10-5)7(3)11/h4H,1-3H3
InchiKey:	JFUVDGXTDCVGHA-UHFFFAOYSA-N
Formula:	C8H10N2O
SMILES:	CC(=O)c1nc(C)cnc1C
Mol. weight [g/mol]:	150.18
CAS:	54300-09-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.61		Crippen Method
logp	1.296		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
rinpol	1144.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1615.00		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=C54300093&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

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