

1-(5-Methyl-2-pyrazinyl)-1-ethanone

Other names:	1-(5-Methyl-2-pyrazinyl)ethanone 1-(5-Methyl-2-pyranizyl)-1-ethanone 2-Acetyl-5-methylpyrazine 2-Methyl-5-acetylpyrazine 5-Methyl-2-acetylpyrazine Pyrazine, 2-acetyl-5-methyl Pyrazine, 5-acetyl-2-methyl
Inchi:	InChI=1S/C7H8N2O/c1-5-3-9-7(4-8-5)6(2)10/h3-4H,1-2H3
InchiKey:	LPQFLJXNMCVMCO-UHFFFAOYSA-N
Formula:	C7H8N2O
SMILES:	CC(=O)c1cnc(C)cn1
Mol. weight [g/mol]:	136.15
CAS:	22047-27-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.14		Crippen Method
logp	0.988		Crippen Method
mcvol	107.260	ml/mol	McGowan Method
rinpol	1088.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1714.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1679.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22047274&Units=SI
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

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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