1-(6-Methyl-2-pyrazinyl)-1-ethanone

Other names:	1-(6-Methyl-2-pyrazinyl)ethanone
	1-(6-Methyl-2-pyranizyl)-1-ethanone
	2-Acetyl-6-methylpyrazine
	2-Methyl-6-acetylpyrazine
	6-Methyl-2-acetylpyrazine
	Pyrazine, 2-acetyl-6-methyl
	Pyrazine, 6-acetyl-2-methyl
Inchi:	InChI=1S/C7H8N2O/c1-5-3-8-4-7(9-5)6(2)10/h3-4H,1-2H3
InchiKey:	YVSDZDUKXQLFLV-UHFFFAOYSA-N
Formula:	C7H8N2O
SMILES:	CC(=O)c1cncc(C)n1
Mol. weight [g/mol]:	136.15
CAS:	22047-26-3

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	1083.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1095.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1679.00		NIST Webbook
ripol	1694.00		NIST Webbook
ripol	1688.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22047263&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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