

2-Acetyl-3-methylpyrazine

Other names:	Ethanone, 1-(3-methylpyrazinyl)- 1-(3-Methyl-2-pyrazinyl)ethanone 1-[3-Methyl-2-pyrazinyl]-1-ethanone 3-Acetyl-2-methylpyrazine Pyrazine, 2-acetyl-3-methyl Pyrazine, 3-acetyl-2-methyl 1-(3-methylpyrazinyl)ethan-1-one
Inchi:	InChI=1S/C7H8N2O/c1-5-7(6(2)10)9-4-3-8-5/h3-4H,1-2H3
InchiKey:	QUNOTZOHYZZWKQ-UHFFFAOYSA-N
Formula:	C7H8N2O
SMILES:	CC(=O)c1nccnc1C
Mol. weight [g/mol]:	136.15
CAS:	23787-80-6

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	1080.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1128.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1112.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1061.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1082.00		NIST Webbook
ripol	1628.00		NIST Webbook
ripol	1640.00		NIST Webbook
ripol	1630.00		NIST Webbook
ripol	1615.00		NIST Webbook
ripol	1635.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1627.00		NIST Webbook

ripol	1635.00	NIST Webbook
ripol	1635.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C23787806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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