

# 2-Acetyl-3-ethylpyrazine

<b>Other names:</b>	Ethanone, 1-(3-ethylpyrazinyl)- 1-(3-Ethyl-2-pyrazinyl)ethanone 2-Ethyl-3-acetyl pyrazine 3-Ethyl-2-acetylpyrazine Pyrazine, 2-acetyl-3-ethyl 1-(3-ethylpyrazinyl)ethan-1-one
<b>Inchi:</b>	InChI=1S/C8H10N2O/c1-3-7-8(6(2)11)10-5-4-9-7/h4-5H,3H2,1-2H3
<b>InchiKey:</b>	PPJSYGVFDJEMRP-UHFFFAOYSA-N
<b>Formula:</b>	C8H10N2O
<b>SMILES:</b>	CCc1nccnc1C(C)=O
<b>Mol. weight [g/mol]:</b>	150.18
<b>CAS:</b>	32974-92-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.47		Crippen Method
logp	1.242		Crippen Method
mcvol	121.350	ml/mol	McGowan Method
rinpol	1172.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1170.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1167.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1617.00		NIST Webbook
ripol	1617.00		NIST Webbook

# Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C32974928&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C32974928&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

# Legend

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

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