Ethanone, 1-(3,5-dimethylpyrazinyl)-

Other names:	2-Acetyl-3,5-dimethylpyrazine
	1-(3,5-Dimethyl-2-pyrazinyl)-1-ethanone
	Pyrazine, 2-acetyl-3,5-dimethyl
	1-(3,5-dimethylpyrazinyl)ethan-1-one
Inchi:	InChI=1S/C8H10N2O/c1-5-4-9-8(7(3)11)6(2)10-5/h4H,1-3H3
InchiKey:	UCGOSAWBWFUKDT-UHFFFAOYSA-N
Formula:	C8H10N2O
SMILES:	CC(=O)c1ncc(C)nc1C
Mol. weight [g/mol]:	150.18
CAS:	54300-08-2

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	1153.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1174.00		NIST Webbook
rinpol	1153.00		NIST Webbook
rinpol	1153.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1629.00		NIST Webbook
ripol	1654.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54300082&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

Latest version available from:
https://www.chemeo.com/cid/63-368-4/Ethanone-1-3-5-dimethylpyrazinyl.pdf
Generated by Cheméo on 2025-12-05 11:36:57.477352693 +0000 UTC m=+4682815.007393356.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.