

Pyrazine, 2-ethyl-3,5-dimethyl-

Other names:	2-Ethyl-3,5-dimethylpyrazine Pyrazine, 3,5-dimethyl-2-ethyl- FEMA 3150 Pyrazine, 2,6-dimethyl-3-ethyl- 2,6-Dimethyl-3-ethylpyrazine 3,5-Dimethyl-2-ethylpyrazine 3-Ethyl-2,6-dimethylpyrazine Pyrazine, 3-ethyl-2,6-dimethyl 2-Ethyl-3,5(6)-dimethylpyrazine
Inchi:	InChI=1S/C8H12N2/c1-4-8-7(3)10-6(2)5-9-8/h5H,4H2,1-3H3
InchiKey:	JZBCTZLGKSYRSF-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CCc1ncc(C)nc1C
Mol. weight [g/mol]:	136.19
CAS:	13925-07-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.76		Crippen Method
logp	1.656		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
rinpol	1068.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1093.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1070.00		NIST Webbook
rinpol	1079.00		NIST Webbook
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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=C13925070&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

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