

2,3-Dimethyl-5-ethylpyrazine

Other names:	2,3-dimethyl-6-ethylpyrazine 2-ethyl-5,6-dimethylpyrazine 5,6-Dimethyl-2-ethylpyrazine 6-Ethyl-2,3-dimethylpyrazine Pyrazine, 6-ethyl-2,3-dimethyl 5-Ethyl-2,3-dimethylpyrazine
Inchi:	InChI=1S/C8H12N2/c1-4-8-5-9-6(2)7(3)10-8/h5H,4H2,1-3H3
InchiKey:	CIBKSMZEVHTQLG-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CCc1cnc(C)c(C)n1
Mol. weight [g/mol]:	136.19
CAS:	15707-34-3

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	1084.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1094.00		NIST Webbook
rinpol	1065.00		NIST Webbook
rinpol	1068.00		NIST Webbook
rinpol	1105.00		NIST Webbook
rinpol	1097.00		NIST Webbook
rinpol	1069.00		NIST Webbook
rinpol	1057.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1090.00		NIST Webbook
rinpol	1096.00		NIST Webbook
rinpol	1066.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1089.00		NIST Webbook

rinpol	1057.00	NIST Webbook
rinpol	1097.00	NIST Webbook
rinpol	1084.00	NIST Webbook
ripol	1460.00	NIST Webbook
ripol	1445.00	NIST Webbook
ripol	1445.00	NIST Webbook
ripol	1470.00	NIST Webbook
ripol	1493.00	NIST Webbook
ripol	1421.00	NIST Webbook
ripol	1447.00	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C15707343&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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