

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

Other names:	2-Ethyl-3,6-dimethylpyrazine 2,5-Dimethyl-3-ethylpyrazine 3-Ethyl-2,5-dimethylpyrazine 3,6-Dimethyl-2-ethylpyrazine Pyrazine, 2-ethyl-3,6-dimethyl
Inchi:	InChI=1S/C8H12N2/c1-4-8-7(3)9-5-6(2)10-8/h5H,4H2,1-3H3
InchiKey:	WHMWOHBXYIZFPF-UHFFFAOYSA-N
Formula:	C8H12N2
SMILES:	CCc1nc(C)cnc1C
Mol. weight [g/mol]:	136.19
CAS:	13360-65-1

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	1078.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1079.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1091.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1084.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1088.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1063.00		NIST Webbook
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ripol	1433.00	NIST Webbook
ripol	1400.00	NIST Webbook
ripol	1455.00	NIST Webbook
ripol	1431.00	NIST Webbook

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13360651&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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