

Pyrazine, 2-methyl-6-(2-propenyl)-

Other names:	2-Allyl-6-methylpyrazine
Inchi:	InChI=1S/C8H10N2/c1-3-4-8-6-9-5-7(2)10-8/h3,5-6H,1,4H2,2H3
InchiKey:	QMVGUEIAPNPNMZ-UHFFFAOYSA-N
Formula:	C8H10N2
SMILES:	C=CCc1cncc(C)n1
Mol. weight [g/mol]:	134.18
CAS:	55138-64-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	1.514		Crippen Method
mcvol	115.480	ml/mol	McGowan Method
rinpol	1170.00		NIST Webbook
rinpol	1074.00		NIST Webbook
rinpol	1170.00		NIST Webbook
ripol	1535.00		NIST Webbook
ripol	1535.00		NIST Webbook

Sources

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=C55138642&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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