

Pyrazine, 2-methyl-5-(2-propenyl)-

Other names:	2-Allyl-5-methylpyrazine
Inchi:	InChI=1S/C8H10N2/c1-3-4-8-6-9-7(2)5-10-8/h3,5-6H,1,4H2,2H3
InchiKey:	JCZDTOUEQCNMKI-UHFFFAOYSA-N
Formula:	C8H10N2
SMILES:	C=CCc1cnc(C)cn1
Mol. weight [g/mol]:	134.18
CAS:	55138-63-1

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	1074.00		NIST Webbook
rinpol	1090.00		NIST Webbook
ripol	1535.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55138631&Units=SI
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

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.cheméo.com/cid/13-887-3/Pyrazine-2-methyl-5-2-propenyl.pdf>

Generated by Cheméo on 2024-04-27 05:19:24.167307062 +0000 UTC m=+16484413.087884373.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.