Pyrazine, (1-methylethenyl)-

Other names:	Isopropenylpyrazine
	2-Isopropenylpyrazine
	(1-Methylethenyl)pyrazine
Inchi:	InChI=1S/C7H8N2/c1-6(2)7-5-8-3-4-9-7/h3-5H,1H2,2H3
InchiKey:	JMKUTMOIKCXELD-UHFFFAOYSA-N
Formula:	C7H8N2
SMILES:	C=C(C)c1cnccn1
Mol. weight [g/mol]:	120.15
CAS:	38713-41-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	1.510		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
rinpol	1092.00		NIST Webbook
rinpol	1042.00		NIST Webbook
rinpol	1028.00		NIST Webbook
rinpol	1075.00		NIST Webbook
rinpol	1021.00		NIST Webbook
rinpol	1083.00		NIST Webbook
rinpol	1045.00		NIST Webbook
rinpol	1092.00		NIST Webbook
rinpol	1021.00		NIST Webbook
ripol	1543.00		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=C38713416&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