

Pyrazine, 2-ethenyl-5-methyl-

Other names:	Pyrazine, 2-methyl-5-vinyl- 2-Methyl-5-vinylpyrazine 2-Ethenyl-5-methyl pyrazine 2-Methyl-5-ethenylpyrazine 2-Vinyl-5-methylpyrazine Pyrazine, 2-vinyl,5-methyl
Inchi:	InChI=1S/C7H8N2/c1-3-7-5-8-6(2)4-9-7/h3-5H,1H2,2H3
InchiKey:	JASFBLBUHWKFBZ-UHFFFAOYSA-N
Formula:	C7H8N2
SMILES:	C=Cc1cnc(C)cn1
Mol. weight [g/mol]:	120.15
CAS:	13925-08-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.30		Crippen Method
logp	1.428		Crippen Method
mcvol	101.390	ml/mol	McGowan Method
rinpol	1037.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	1034.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1032.00		NIST Webbook
rinpol	1035.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	1031.00		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	994.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1025.00		NIST Webbook
rinpol	1022.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	1023.00		NIST Webbook

ripol	1023.00	NIST Webbook
ripol	1041.00	NIST Webbook
ripol	1488.00	NIST Webbook
ripol	1493.00	NIST Webbook
ripol	1476.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1538.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1513.00	NIST Webbook
ripol	1489.00	NIST Webbook
ripol	1520.00	NIST Webbook
ripol	1529.00	NIST Webbook
ripol	1498.00	NIST Webbook
ripol	1500.00	NIST Webbook
ripol	1485.00	NIST Webbook
ripol	1495.00	NIST Webbook
ripol	1516.00	NIST Webbook
ripol	1520.00	NIST Webbook
ripol	1476.00	NIST Webbook
ripol	1468.00	NIST Webbook
ripol	1485.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13925081&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
ripol:	Non-polar retention indices
ripol:	Polar retention indices

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