

Pyrazine, 2-ethyl-6-methyl-

Other names:	2-Ethyl-6-methylpyrazine 2-Methyl-6-ethylpyrazine 2,6-Methylethylpyrazine Pyrazine, 6-ethyl-2-methyl
Inchi:	InChI=1S/C7H10N2/c1-3-7-5-8-4-6(2)9-7/h4-5H,3H2,1-2H3
InchiKey:	RAFHQTNQEZEZCFL-UHFFFAOYSA-N
Formula:	C7H10N2
SMILES:	CCc1cncc(C)n1
Mol. weight [g/mol]:	122.17
CAS:	13925-03-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.28		Crippen Method
logp	1.347		Crippen Method
mcvol	105.690	ml/mol	McGowan Method
rinpol	997.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	1003.00		NIST Webbook
rinpol	1011.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	1001.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	970.00		NIST Webbook
rinpol	969.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	959.00		NIST Webbook

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rinpol	988.00	NIST Webbook
rinpol	1006.00	NIST Webbook
rinpol	995.00	NIST Webbook
rinpol	1000.00	NIST Webbook
rinpol	1003.00	NIST Webbook
rinpol	994.00	NIST Webbook
rinpol	1014.00	NIST Webbook
rinpol	998.00	NIST Webbook
rinpol	970.00	NIST Webbook
rinpol	1001.00	NIST Webbook
rinpol	982.00	NIST Webbook
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rinpol	994.00	NIST Webbook
rinpol	1012.00	NIST Webbook
rinpol	1009.00	NIST Webbook
rinpol	1008.00	NIST Webbook
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ripol	1380.00	NIST Webbook
ripol	1413.00	NIST Webbook
ripol	1402.00	NIST Webbook
ripol	1387.00	NIST Webbook
ripol	1386.00	NIST Webbook
ripol	1386.00	NIST Webbook
ripol	1371.00	NIST Webbook
ripol	1381.00	NIST Webbook
ripol	1390.00	NIST Webbook
ripol	1390.00	NIST Webbook
ripol	1386.00	NIST Webbook
ripol	1375.00	NIST Webbook
ripol	1371.00	NIST Webbook
ripol	1395.00	NIST Webbook
ripol	1395.00	NIST Webbook
ripol	1385.00	NIST Webbook
ripol	1381.00	NIST Webbook
ripol	1393.00	NIST Webbook
ripol	1363.00	NIST Webbook

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C13925036&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

https://www.cheméo.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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