

Pyrazine, ethenyl-

Other names:	Pyrazine, vinyl- Vinylpyrazine 2-Vinylpyrazine Ethenylpyrazine
Inchi:	InChI=1S/C6H6N2/c1-2-6-5-7-3-4-8-6/h2-5H,1H2
InchiKey:	KANZWHBYRHQMKZ-UHFFFAOYSA-N
Formula:	C6H6N2
SMILES:	C=Cc1cnccn1
Mol. weight [g/mol]:	106.13
CAS:	4177-16-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.83		Crippen Method
logp	1.120		Crippen Method
mcvol	87.300	ml/mol	McGowan Method
rinpol	947.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	900.00		NIST Webbook
rinpol	908.00		NIST Webbook
rinpol	909.00		NIST Webbook
rinpol	922.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	901.00		NIST Webbook
rinpol	923.00		NIST Webbook
rinpol	912.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	926.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	946.00		NIST Webbook
rinpol	954.00		NIST Webbook
rinpol	905.00		NIST Webbook
rinpol	950.00		NIST Webbook

ripol	907.00	NIST Webbook
ripol	907.00	NIST Webbook
ripol	907.00	NIST Webbook
ripol	946.00	NIST Webbook
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ripol	1434.00	NIST Webbook
ripol	1422.00	NIST Webbook
ripol	1413.00	NIST Webbook
ripol	1467.00	NIST Webbook
ripol	1449.00	NIST Webbook
ripol	1392.00	NIST Webbook
ripol	1449.00	NIST Webbook
ripol	1415.00	NIST Webbook
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ripol	1429.00	NIST Webbook
ripol	1436.00	NIST Webbook
ripol	1436.00	NIST Webbook
ripol	1467.00	NIST Webbook
ripol	1467.00	NIST Webbook
ripol	1467.00	NIST Webbook
ripol	1447.00	NIST Webbook
ripol	1447.00	NIST Webbook
ripol	1413.00	NIST Webbook
ripol	1416.00	NIST Webbook
ripol	1438.00	NIST Webbook
ripol	1438.00	NIST Webbook
ripol	1438.00	NIST Webbook
ripol	1434.00	NIST Webbook

Sources

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C4177166&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices

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