

1H-Pyrrole, 1-(2-furanylmethyl)-

Other names:	1-(2-Furanylmethyl)-1H-pyrrole 1-Furfurylpyrrole N-Furfurylpyrrole Pyrrole, 1-furfuryl- N-(2-Furfuryl)pyrrole 1-(2-Furanmethyl)-1H-pyrrole 1-(2-Furfuryl)pyrrole 1-(2-Furfuryl)-1H-pyrrole 1-(2-Furfuryl)-pyrrole 1H-Pyrrole, 1-(2-furfuryl) 2-Furfurylpyrrole 1-(2-furanylmethyl)-1H-pyrrole (furfurylpyrrole) 1-Furfuryl-1H-pyrrol 1-furfuryl-1H-pyrrole
Inchi:	InChI=1S/C9H9NO/c1-2-6-10(5-1)8-9-4-3-7-11-9/h1-7H,8H2
InchiKey:	BTBFUBUCCJKJOZ-UHFFFAOYSA-N
Formula:	C9H9NO
SMILES:	c1coc(Cn2cccc2)c1
Mol. weight [g/mol]:	147.17
CAS:	1438-94-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.76		Crippen Method
logp	2.129		Crippen Method
mcvol	114.600	ml/mol	McGowan Method
rinpol	1185.40		NIST Webbook
rinpol	1149.00		NIST Webbook
rinpol	1195.00		NIST Webbook
rinpol	1151.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1185.40		NIST Webbook
rinpol	1182.00		NIST Webbook
rinpol	1196.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1189.00		NIST Webbook
rinpol	1197.00		NIST Webbook

ripol	1155.00	NIST Webbook
ripol	1182.00	NIST Webbook
ripol	1163.00	NIST Webbook
ripol	1133.00	NIST Webbook
ripol	1162.00	NIST Webbook
ripol	1148.00	NIST Webbook
ripol	1183.00	NIST Webbook
ripol	1166.00	NIST Webbook
ripol	1195.00	NIST Webbook
ripol	1189.00	NIST Webbook
ripol	1133.00	NIST Webbook
ripol	1172.00	NIST Webbook
ripol	1833.00	NIST Webbook
ripol	1820.00	NIST Webbook
ripol	1838.00	NIST Webbook
ripol	1822.00	NIST Webbook
ripol	1824.00	NIST Webbook
ripol	1821.00	NIST Webbook
ripol	1823.00	NIST Webbook
ripol	1824.00	NIST Webbook
ripol	1858.00	NIST Webbook
ripol	1817.00	NIST Webbook
ripol	1850.00	NIST Webbook
ripol	1824.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	350.20	K	0.10	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=C1438944&Units=SI>
- Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
tbrp:	Boiling point at reduced pressure

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