Furan, 3-methyl-

Other names:	3-Methylfuran
	3-Methylfurane
Inchi:	InChI=1S/C5H6O/c1-5-2-3-6-4-5/h2-4H,1H3
InchiKey:	KJRRQXYWFQKJIP-UHFFFAOYSA-N
Formula:	C5H6O
SMILES:	Cc1ccoc1
Mol. weight [g/mol]:	82.10
CAS:	930-27-8

Physical Properties

Property code	Value	Unit	Source
affp	854.00	kJ/mol	NIST Webbook
basg	821.50	kJ/mol	NIST Webbook
ie	8.58	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
ie	8.64	eV	NIST Webbook
log10ws	-5.68		Crippen Method
logp	1.588		Crippen Method
mcvol	67.720	ml/mol	McGowan Method
rinpol	611.10		NIST Webbook
rinpol	620.00		NIST Webbook
rinpol	602.20		NIST Webbook
rinpol	603.00		NIST Webbook
rinpol	602.96		NIST Webbook
rinpol	614.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	602.00		NIST Webbook
rinpol	646.00		NIST Webbook
rinpol	600.00		NIST Webbook
ripol	854.00		NIST Webbook
ripol	851.00		NIST Webbook
ripol	877.00		NIST Webbook
ripol	877.00		NIST Webbook
ripol	901.00		NIST Webbook
ripol	832.00		NIST Webbook
ripol	832.00		NIST Webbook
ripol	858.00		NIST Webbook

ripol	854.00	NIST Webbook
ripol	854.00	NIST Webbook
ripol	853.00	NIST Webbook
ripol	853.00	NIST Webbook
ripol	852.00	NIST Webbook
ripol	851.00	NIST Webbook
ripol	851.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55175e+01
Coeff. B	-3.24588e+03
Coeff. C	-3.52950e+01
Temperature range (K), min.	248.42
Temperature range (K), max.	353.33

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C930278&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

pvap: Vapor pressure
rinpol: Non-polar retention indices
ripol: Polar retention indices