

# Furan, 2-ethyl-5-methyl-

<b>Other names:</b>	2-Ethyl-5-methylfuran 2-Methyl-5-ethylfuran furan, 2-methyl, 5-ethyl
<b>Inchi:</b>	InChI=1S/C7H10O/c1-3-7-5-4-6(2)8-7/h4-5H,3H2,1-2H3
<b>InchiKey:</b>	NBXLPPVOZWYADY-UHFFFAOYSA-N
<b>Formula:</b>	C7H10O
<b>SMILES:</b>	CCc1ccc(C)o1
<b>Mol. weight [g/mol]:</b>	110.15
<b>CAS:</b>	1703-52-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-6.48		Crippen Method
logp	2.150		Crippen Method
mcvol	95.900	ml/mol	McGowan Method
rinpol	799.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	810.00		NIST Webbook
rinpol	771.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	789.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	791.00		NIST Webbook
rinpol	802.00		NIST Webbook
rinpol	797.00		NIST Webbook
rinpol	799.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	803.00		NIST Webbook

ripol	1028.00	NIST Webbook
ripol	1012.00	NIST Webbook
ripol	1013.00	NIST Webbook
ripol	1014.00	NIST Webbook
ripol	1015.00	NIST Webbook
ripol	1015.00	NIST Webbook
ripol	1018.00	NIST Webbook
ripol	1014.00	NIST Webbook
ripol	1032.00	NIST Webbook
ripol	1034.00	NIST Webbook
ripol	1034.00	NIST Webbook
ripol	1014.00	NIST Webbook
ripol	1024.00	NIST Webbook
ripol	1013.00	NIST Webbook
ripol	1013.00	NIST Webbook
ripol	1024.00	NIST Webbook
ripol	1028.00	NIST Webbook
ripol	1015.00	NIST Webbook
ripol	1032.00	NIST Webbook

## Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51727e+01
Coeff. B	-3.58420e+03
Coeff. C	-5.00290e+01
Temperature range (K), min.	290.82
Temperature range (K), max.	413.49

## Sources

The Yaws Handbook of Vapor Pressure:  
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>  
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C1703522&Units=SI>

# Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pvap:</b>	Vapor pressure
<b>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</b>	Polar retention indices

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