

# 2,3-dimethylfuran

Inchi:	InChI=1S/C6H8O/c1-5-3-4-7-6(5)2/h3-4H,1-2H3
InchiKey:	FJSKXQVRKZTKSI-UHFFFAOYSA-N
Formula:	C6H8O
SMILES:	Cc1ccoc1C
Mol. weight [g/mol]:	96.13
CAS:	14920-89-9

## Physical Properties

Property code	Value	Unit	Source
ie	8.00	eV	NIST Webbook
ie	8.25 ± 0.10	eV	NIST Webbook
log10ws	-6.16		Crippen Method
logp	1.896		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	725.00		NIST Webbook
rinpol	705.00		NIST Webbook
rinpol	725.00		NIST Webbook
ripol	953.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	955.00		NIST Webbook
ripol	953.00		NIST Webbook
ripol	954.00		NIST Webbook
tb	367.65 ± 2.00	K	NIST Webbook
tb	363.65 ± 2.00	K	NIST Webbook

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	360.20	K	96.00	NIST Webbook
tbrp	315.20	K	15.30	NIST Webbook

# Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49125e+01
Coeff. B	-3.33832e+03
Coeff. C	-4.33570e+01
Temperature range (K), min.	271.62
Temperature range (K), max.	391.06

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C14920899&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14920899&amp;Units=SI</a>
<b>The Yaws Handbook of Vapor Pressure:</b>	<a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>ie:</b>	Ionization energy
<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>rinpola:</b>	Non-polar retention indices
<b>ripola:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure

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