

2,4-Dimethylfuran

Other names:	Furan, 2,4-dimethyl-
Inchi:	InChI=1S/C6H8O/c1-5-3-6(2)7-4-5/h3-4H,1-2H3
InchiKey:	AABTWRKUKUPMJG-UHFFFAOYSA-N
Formula:	C6H8O
SMILES:	Cc1coc(C)c1
Mol. weight [g/mol]:	96.13
CAS:	3710-43-8

Physical Properties

Property code	Value	Unit	Source
affp	894.70	kJ/mol	NIST Webbook
basg	862.30	kJ/mol	NIST Webbook
ie	8.39 ± 0.10	eV	NIST Webbook
log10ws	-6.16		Crippen Method
logp	1.896		Crippen Method
mcvol	81.810	ml/mol	McGowan Method
rinpol	703.00		NIST Webbook
rinpol	708.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	706.00		NIST Webbook
rinpol	735.00		NIST Webbook
rinpol	704.00		NIST Webbook
rinpol	729.00		NIST Webbook
rinpol	695.00		NIST Webbook
ripol	949.00		NIST Webbook
ripol	958.00		NIST Webbook
ripol	954.00		NIST Webbook
ripol	949.00		NIST Webbook
ripol	936.00		NIST Webbook
ripol	943.00		NIST Webbook
ripol	944.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	948.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	945.00		NIST Webbook
ripol	978.00		NIST Webbook

tb	367.15 ± 2.00	K	NIST Webbook
tb	368.65 ± 2.00	K	NIST Webbook
tb	368.25 ± 0.60	K	NIST Webbook
tb	367.90 ± 0.50	K	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50217e+01
Coeff. B	-3.36711e+03
Coeff. C	-4.34960e+01
Temperature range (K), min.	272.02
Temperature range (K), max.	390.25

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3710438&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

tb: Normal Boiling Point Temperature

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