

# Methyl 2-furoate

<b>Other names:</b>	2-Furancarboxylic acid, methyl ester 2-Furoic acid, methyl ester Methyl pyromucate Methyl 2-furancarboxylate Pyromucic acid methyl ester Methyl «alpha»-furoate Furan-«alpha»-carboxylic acid methyl ester 2-(Methoxycarbonyl)furan Methyl 2-furylcarboxylate NSC 35551 Methyl furoate
<b>Inchi:</b>	InChI=1S/C6H6O3/c1-8-6(7)5-3-2-4-9-5/h2-4H,1H3
<b>InchiKey:</b>	HDJLSECJEQSPKW-UHFFFAOYSA-N
<b>Formula:</b>	C6H6O3
<b>SMILES:</b>	COC(=O)c1ccco1
<b>Mol. weight [g/mol]:</b>	126.11
<b>CAS:</b>	611-13-2

## Physical Properties

Property code	Value	Unit	Source
chl	-2769.00 ± 0.40	kJ/mol	NIST Webbook
hf	-405.00 ± 2.00	kJ/mol	NIST Webbook
hfl	-450.20 ± 0.40	kJ/mol	NIST Webbook
hvap	45.20	kJ/mol	NIST Webbook
hvap	45.20 ± 0.80	kJ/mol	NIST Webbook
ie	9.00 ± 0.05	eV	NIST Webbook
ie	9.32 ± 0.05	eV	NIST Webbook
log10ws	-5.45		Crippen Method
logp	1.066		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
rinpola	978.00		NIST Webbook
rinpola	972.00		NIST Webbook
rinpola	975.00		NIST Webbook
rinpola	956.00		NIST Webbook
rinpola	981.00		NIST Webbook
rinpola	984.90		NIST Webbook
rinpola	978.00		NIST Webbook

ripol	976.00			NIST Webbook
ripol	937.00			NIST Webbook
ripol	956.00			NIST Webbook
ripol	950.00			NIST Webbook
ripol	983.00			NIST Webbook
ripol	978.00			NIST Webbook
ripol	984.90			NIST Webbook
ripol	950.00			NIST Webbook
ripol	983.00			NIST Webbook
ripol	983.00			NIST Webbook
ripol	980.00			NIST Webbook
ripol	983.00			NIST Webbook
ripol	985.00			NIST Webbook
ripol	1561.00			NIST Webbook
ripol	1569.00			NIST Webbook
ripol	1562.00			NIST Webbook
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ripol	1565.00			NIST Webbook
ripol	1567.00			NIST Webbook
ripol	1515.00			NIST Webbook
ripol	1557.00			NIST Webbook
ripol	1578.00			NIST Webbook
ripol	1561.00			NIST Webbook
ripol	1558.00			NIST Webbook
ripol	1561.00			NIST Webbook
ripol	1570.00			NIST Webbook
ripol	1572.00			NIST Webbook
ripol	1558.00			NIST Webbook
ripol	1563.00			NIST Webbook
ripol	1562.00			NIST Webbook
ripol	1567.00			NIST Webbook
ripol	1553.00			NIST Webbook
ripol	1572.00			NIST Webbook
ripol	1561.00			NIST Webbook
tb	454.50		K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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## Sources

<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>
<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=C611132&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C611132&amp;Units=SI</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfl:</b>	Liquid phase enthalpy of formation at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>rinpola:</b>	Non-polar retention indices
<b>ripola:</b>	Polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature

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