Methyl 2-furoate

Other names:	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
Inchi:	InChI=1S/C6H6O3/c1-8-6(7)5-3-2-4-9-5/h2-4H,1H3
InchiKey:	HDJLSECJEQSPKW-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	COC(=O)c1ccco1
Mol. weight [g/mol]:	126.11
CAS:	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 ± 0.80	kJ/mol	NIST Webbook
hvap	45.20	kJ/mol	NIST Webbook
ie	9.32 ± 0.05	eV	NIST Webbook
ie	9.00 ± 0.05	eV	NIST Webbook
log10ws	-5.45		Crippen Method
logp	1.066		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
rinpol	983.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	937.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	985.00		NIST Webbook

rinpol	981.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	984.90		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	984.90		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1572.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1570.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1558.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1578.00		NIST Webbook
ripol	1557.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1567.00		NIST Webbook
ripol	1565.00		NIST Webbook
ripol	1564.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1563.00		NIST Webbook
ripol	1562.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1561.00		NIST Webbook
ripol	1553.00		NIST Webbook
ripol	1572.00		NIST Webbook
ripol	1563.00		NIST Webbook
tb	454.50	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

hvapt	44.43	kJ/mol	454.80	NIST Webbook

Sources

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=C611132&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature