2,5-Furandione, 3,4-dimethyl-

Other names:	Maleic anhydride, dimethyl-
	Dimethylmaleic acid anhydride
	Dimethylmaleic anhydride
	Pyrocinchonic anhydride
	2,3-Dimethylmaleic anhydride
	3,4-Dimethyl-2,5-furandione
	«alpha»,«beta»-Dimethylmaleic anhydride
	Anhydride of dimethylmaleic acid
	3,4-Dimethyl-2,5-furanedione
	NSC 92512
Inchi:	InChI=1S/C6H6O3/c1-3-4(2)6(8)9-5(3)7/h1-2H3
InchiKey:	MFGALGYVFGDXIX-UHFFFAOYSA-N
Formula:	C6H6O3
SMILES:	CC1=C(C)C(=O)OC1=O
Mol. weight [g/mol]:	126.11
CAS:	766-39-2

Physical Properties

Property code	Value	Unit	Source
chs	-2637.20 ± 2.50	kJ/mol	NIST Webbook
ea	1.16 ± 0.09	eV	NIST Webbook
gf	-276.70	kJ/mol	Joback Method
hf	-458.91	kJ/mol	Joback Method
hfs	-574.50	kJ/mol	NIST Webbook
hfus	11.60	kJ/mol	Joback Method
hvap	44.14	kJ/mol	Joback Method
log10ws	-0.72		Crippen Method
logp	0.406		Crippen Method
mcvol	89.250	ml/mol	McGowan Method
pc	4362.63	kPa	Joback Method
rinpol	996.00		NIST Webbook
rinpol	1038.00		NIST Webbook
rinpol	1038.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1764.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1714.00		NIST Webbook

ripol	1764.00		NIST Webbook
ripol	1680.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1685.00		NIST Webbook
ripol	1755.00		NIST Webbook
ripol	1688.00		NIST Webbook
tb	496.20	K	NIST Webbook
tc	768.10	K	Joback Method
tf	361.33	K	Joback Method
vc	0.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.56	J/mol×K	528.34	Joback Method
cpg	205.91	J/mol×K	568.30	Joback Method
cpg	215.95	J/mol×K	608.26	Joback Method
cpg	225.63	J/mol×K	648.22	Joback Method
cpg	234.88	J/mol×K	688.18	Joback Method
cpg	243.64	J/mol×K	728.14	Joback Method
cpg	251.87	J/mol×K	768.10	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C766392&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
ea: Electron affinity
gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume