2,5-Furandione, 3-methyl-

Other names:	Citraconic anhydride
	«alpha»-Methylmaleic anhydride
	Citraconic acid anhydride
	Methylmaleic anhydride
	Monomethylmaleic anhydride
	2-Methylmaleic anhydride
	3-Methylmaleic anhydride
	3-Methyl-2,5-furandione
	Maleic anhydride, methyl-
	Anhydrid kyseliny citrakonove
	2,5-Furanedione, 3-methyl
	NSC 6182
Inchi:	InChI=1S/C5H4O3/c1-3-2-4(6)8-5(3)7/h2H,1H3
InchiKey:	AYKYXWQEBUNJCN-UHFFFAOYSA-N
Formula:	C5H4O3
SMILES:	CC1=CC(=O)OC1=O
Mol. weight [g/mol]:	112.08
CAS:	616-02-4

Physical Properties

Property code	Value	Unit	Source
gf	-275.49	kJ/mol	Joback Method
hf	-426.80	kJ/mol	Joback Method
hfus	9.40	kJ/mol	Joback Method
hvap	41.25	kJ/mol	Joback Method
ie	10.95	eV	NIST Webbook
ie	10.70	eV	NIST Webbook
log10ws	-0.30		Crippen Method
logp	0.016		Crippen Method
mcvol	75.160	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
rinpol	941.00		NIST Webbook
rinpol	941.00		NIST Webbook
rinpol	949.00		NIST Webbook
rinpol	949.00		NIST Webbook
tb	486.70	K	NIST Webbook
tc	743.72	K	Joback Method

tf	279.65 ± 1.50	K	NIST Webbook
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.49	J/mol×K	500.48	Joback Method
cpg	164.63	J/mol×K	541.02	Joback Method
cpg	173.51	J/mol×K	581.56	Joback Method
cpg	182.10	J/mol×K	622.10	Joback Method
cpg	190.32	J/mol×K	662.64	Joback Method
cpg	198.13	J/mol×K	703.18	Joback Method
cpg	205.47	J/mol×K	743.72	Joback Method
hvapt	53.30	kJ/mol	403.50	NIST Webbook

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=C616024&Units=SI

Legend

cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion 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

pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume