2,5-Furandione, dihydro-3-methyl-

Other names:	Succinic anhydride, methyl-
	Methylsuccinic anhydride
	Pyrotartaric anhydride
	2-Methylsuccinic anhydride
	3-Methylsuccinic anhydride
	3,4-Dihydro-3-methyl-2,5-furandione
	3-Methyldihydro-2,5-furandione
Inchi:	InChI=1S/C5H6O3/c1-3-2-4(6)8-5(3)7/h3H,2H2,1H3
InchiKey:	DFATXMYLKPCSCX-UHFFFAOYSA-N
Formula:	C5H6O3
SMILES:	CC1CC(=O)OC1=O
Mol. weight [g/mol]:	114.10
CAS:	4100-80-5

Physical Properties

Property code	Value	Unit	Source
chl	-2213.80 ± 1.10	kJ/mol	NIST Webbook
chs	-2205.10 ± 1.10	kJ/mol	NIST Webbook
gf	-303.53	kJ/mol	Joback Method
hf	-493.45	kJ/mol	Joback Method
hfus	9.64	kJ/mol	Joback Method
hvap	39.98	kJ/mol	Joback Method
log10ws	-0.21		Crippen Method
logp	0.096		Crippen Method
mcvol	79.460	ml/mol	McGowan Method
pc	4710.65	kPa	Joback Method
ripol	1855.00		NIST Webbook
ripol	1855.00		NIST Webbook
tb	512.20	K	NIST Webbook
tc	730.88	K	Joback Method
tf	309.85 ± 1.00	K	NIST Webbook
vc	0.291	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.31	J/mol×K	491.67	Joback Method
cpg	185.67	J/mol×K	531.54	Joback Method
cpg	196.68	J/mol×K	571.41	Joback Method
cpg	207.29	J/mol×K	611.27	Joback Method
cpg	217.44	J/mol×K	651.14	Joback Method
cpg	227.09	J/mol×K	691.01	Joback Method
cpg	236.16	J/mol×K	730.88	Joback Method
hvapt	59.30	kJ/mol	431.50	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4100805&Units=SI
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

Legend

chl: Standard liquid enthalpy of combustion
chs: Standard solid enthalpy of combustion
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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume