

2,5-Furandione, 3,4-dichloro-

Other names:	Maleic anhydride, dichloro- Dichloromaleic acid anhydride Dichloromaleic anhydride 2,3-Dichloromaleic anhydride 2,3-Dichloromaleic acid anhydride
Inchi:	InChI=1S/C4Cl2O3/c5-1-2(6)4(8)9-3(1)7
InchiKey:	AGULWIIQYWWFBJ-UHFFFAOYSA-N
Formula:	C4Cl2O3
SMILES:	O=C1OC(=O)C(Cl)=C1Cl
Mol. weight [g/mol]:	166.95
CAS:	1122-17-4

Physical Properties

Property code	Value	Unit	Source
ea	1.90 ± 0.09	eV	NIST Webbook
gf	-317.40	kJ/mol	Joback Method
hf	-449.11	kJ/mol	Joback Method
hfus	14.82	kJ/mol	Joback Method
hvap	48.45	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	0.759		Crippen Method
mcvol	85.550	ml/mol	McGowan Method
pc	5131.32	kPa	Joback Method
tb	557.44	K	Joback Method
tc	816.61	K	Joback Method
tf	398.63	K	Joback Method
vc	0.321	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.50	J/mol×K	557.44	Joback Method
cpg	158.96	J/mol×K	600.63	Joback Method
cpg	165.22	J/mol×K	643.83	Joback Method

cpg	171.21	J/mol×K	687.02	Joback Method
cpg	176.84	J/mol×K	730.22	Joback Method
cpg	182.05	J/mol×K	773.41	Joback Method
cpg	186.74	J/mol×K	816.61	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1122174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvac:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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