1H-Pyrrole-2,5-dione

Other names:	Maleimide
	Pyrrole-2,5-dione
	3-Pyrroline-2,5-dione
	Maleinimide
	Maleic imide
Inchi:	InChI=1S/C4H3NO2/c6-3-1-2-4(7)5-3/h1-2H,(H,5,6,7)
InchiKey:	PEEHTFAAVSWFBL-UHFFFAOYSA-N
Formula:	C4H3NO2
SMILES:	O=C1C=CC(=O)N1
Mol. weight [g/mol]:	97.07
CAS:	541-59-3

Physical Properties

Property code	Value	Unit	Source
ea	1.15 ± 0.09	eV	NIST Webbook
gf	-100.45	kJ/mol	Joback Method
hf	-224.88	kJ/mol	Joback Method
hfus	8.81	kJ/mol	Joback Method
hvap	40.61	kJ/mol	Joback Method
log10ws	0.01		Crippen Method
logp	-0.801		Crippen Method
mcvol	65.180	ml/mol	McGowan Method
pc	6318.86	kPa	Joback Method
tb	494.22	K	Joback Method
tc	749.10	K	Joback Method
tf	392.21	K	Joback Method
vc	0.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	124.54	J/mol×K	494.22	Joback Method
cpg	133.31	J/mol×K	536.70	Joback Method
cpg	141.86	J/mol×K	579.18	Joback Method

cpg	150.14	J/mol×K	621.66	Joback Method
cpg	158.07	J/mol×K	664.14	Joback Method
cpg	165.59	J/mol×K	706.62	Joback Method
cpg	172.62	J/mol×K	749.10	Joback Method

Sources

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=C541593&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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