N-Methylmaleimide

Other names: 1H-Pyrrole-2,5-dione, 1-methyl-
Maleimide, N-methyl-
N-Methylmaleinimide
Inchi: InChI=1S/C5H5NO2/c1-6-4(7)2-3-5(6)8/h2-3H,1H3
InchiKey: SEEYREPSKCQBBF-UHFFFAOYSA-N
Formula: C5H5NO2
SMILES: CN1C(=O)C=CC1=O
Mol. weight [g/mol]: 111.10
CAS: 930-88-1

Physical Properties

Property code	Value	Unit	Source
chs	-2352.80 ± 1.30	kJ/mol	NIST Webbook
ea	1.11 ± 0.09	eV	NIST Webbook
hf	-256.00 ± 1.50	kJ/mol	NIST Webbook
hfs	-329.30 ± 1.40	kJ/mol	NIST Webbook
hsub	73.30 ± 0.50	kJ/mol	NIST Webbook
hsub	73.30 ± 0.50	kJ/mol	NIST Webbook
log10ws	0.22		Crippen Method
logp	-0.459		Crippen Method
mcvol	79.270	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	75.30 ± 0.50	kJ/mol	282.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C930881&Units=SI

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

Legend

chs:	Standard solid enthalpy of combustion
ea:	Electron affinity
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume