1H-Indole-2,3-dione, 1-methyl-

Other names:	Indole-2,3-dione, 1-methyl-
	N-Methylisatin
	OL 57
	1-Methylisatin
	1-Methyl-indole-2,3-dione
	1-Methyl-2,3-indolinedione
	Indole-2,3-dione, N-methyl-
	1-Methyl-1H-indole-2,3-dione
	NSC 42449
	1-methyl-2,3-dihydroindole-2,3-dione
	1-Methyl-1H-indole-2,3-dione (N-methylisatin)
Inchi:	InChI=1S/C9H7NO2/c1-10-7-5-3-2-4-6(7)8(11)9(10)12/h2-5H,1H3
InchiKey:	VCYBVWFTGAZHGH-UHFFFAOYSA-N
Formula:	C9H7NO2
SMILES:	CN1C(=O)C(=O)c2ccccc21
Mol. weight [g/mol]:	161.16
CAS:	2058-74-4

Physical Properties

Property code	Value	Unit	Source
hsub	105.60 ± 3.30	kJ/mol	NIST Webbook
log10ws	-1.29		Crippen Method
logp	0.846		Crippen Method
mcvol	116.170	ml/mol	McGowan Method
rinpol	1477.00		NIST Webbook
rinpol	1477.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	19.50	kJ/mol	403.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2058744&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices