Indan-1,2,3-trione

Other names:	1H-Indene-1,2,3-trione
	1,2,3-Indantrione
	Indantrione
	1,2,3-Triketohydrindene
Inchi:	InChI=1S/C9H4O3/c10-7-5-3-1-2-4-6(5)8(11)9(7)12/h1-4H
InchiKey:	WVZWEMOFSIEEMU-UHFFFAOYSA-N
Formula:	C9H4O3
SMILES:	O=c1c(=O)c2ccccc2c1=O
Mol. weight [g/mol]:	160.13
CAS:	938-24-9

Physical Properties

Property code	Value	Unit	Source
ie	9.10	eV	NIST Webbook
log10ws	-0.37		Crippen Method
logp	-0.204		Crippen Method
mcvol	107.760	ml/mol	McGowan Method

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=C938249&Units=SI

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume