1H-Pyrrole-2,5-dione, 1-[4-(dimethylamino)-3,5-dinitrophenyl]-

Other names: Maleimide, N-[4-(dimethylamino)-3,5-dinitrophenyl]-
N-(4-Dimethylamino-3,5-dinitrophenyl)maleimide
1-[4-(dimethylamino)-3,5-dinitrophenyl]-1H-pyrrole-2,5-dione

Inchi: InChI=1S/C12H10N4O6/c1-13(2)12-8(15(19)20)5-7(6-9(12)16(21)22)14-10(17)3-4-11(14

InchiKey: QPYAUURPGVXHFK-UHFFFAOYSA-N

Formula: C12H10N4O6

SMILES: CN(C)c1c([N+](=O)[O-])cc(N2C(=O)C=CC2=O)cc1[N+](=O)[O-]

Mol. weight [g/mol]: 306.23

CAS: 3475-74-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	0.998		Crippen Method
mcvol	198.960	ml/mol	McGowan Method

Sources

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=C3475749&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume