

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

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