

Dithianone

Other names:

Naphtho[2,3-b]-1,4-dithiin-2,3-dicarbonitrile, 5,10-dihydro-5,10-dioxo-
Naphtho[2,3-b]-p-dithiin-2,3-dicarbonitrile, 5,10-dihydro-5,10-dioxo-
Delan
Delan WP
Dithianon
Merkdelan
MV 119A
Stauffer MV-119A
Thynon
2,3-Dicyano-1,4-dithiaanthraquinone
2,3-Dinitrilo-1,4-dithiaanthraquinone
Delan-Col
IT 931
1,4-Dithiaanthraquinone-2,3-dinitrile
2,3-Dicarbonitrilo-1,4-diathiaanthrachinon
2,3-Dinitrilo-1,4-dithioanthrachinon
5,10-Dihydro-5,10-dioxonaphtho(2,3-b)-p-dithiin-2,3-dicarbonitrile
5,10-Dihydro-5,10-dioxonaphtho[2,3-b]-1,4-dithiin-2,3-dicarbonitrile
1,4-Dithiaanthraquinone-2,3-dicarbonitrile
2,3-Dinitrilo-1,4-dithia-9,10-anthraquinone
Delan (fungicide)
NSC 218452

Inchi: InChI=1S/C14H4N2O2S2/c15-5-9-10(6-16)20-14-12(18)8-4-2-1-3-7(8)11(17)13(14)19-9/
InchiKey: PYZSVQVRHDXQSL-UHFFFAOYSA-N
Formula: C14H4N2O2S2
SMILES: N#Cc1sc2c(=O)c3ccccc3c(=O)c=2sc1C#N
Mol. weight [g/mol]: 296.32
CAS: 3347-22-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.88		Crippen Method
logp	2.151		Crippen Method
mcpvol	192.640	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3347226&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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

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