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Typical Product Specifications & Properties

1,8-dihydroxy-2,4,5,7-tetranitroanthraquinone

CAS Number: : 517-92-0

Specifications	Limits
Molecular weight	420.20
EINECS	208-246-2
SMILES	<chem>c12c(C(c3c(c([N+](=O)[O-])cc(c3C2=O)[N+](=O)[O-])O)=O)c(c([N+](=O)[O-])cc1[N+](=O)[O-])O</chem>
InChI	YYOOOMNEONKALI-UHFFFAOYSA-N
InChIKey	1S/C14H4N4O12/c19-11-5(17(27)28)1-3(15(23)24)7-9(11)14(22)10-8(13(7)21)4(16(25)26)2-6(12(10)20)18(29)30/h1-2,19-20H
Atmospheric OH Rate Constant	2.88E-13 cm ³ /molecule-sec
log P (octanol-water)	4.360

