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## Typical Product Specifications & Properties

# Methotrexate Dimethyl Ester

CAS Number: : 34378-65-9

Specifications	Limits
Molecular weight	482.49
SMILES	<chem>CN(Cc1cnc2c(n1)c(nc(n2)N)N)c3ccc(cc3)C(=O)N[C@@H](CCC(=O)OC)C(=O)OC</chem>
InChI	DIQFVFAFHNQUTG-HNNXBMFYSA-N
InChIKey	1S/C22H26N8O5/c1-30(11-13-10-25-19-17(26-13)18(23)28-22(24)29-19)14-6-4-12(5-7-14)20(32)27-15(21(33)35-3)8-9-16(31)34-2/h4-7,10,15H,8-9,11H2,1-3H3,(H,27,32)(H4,23,24,25,28,29)/t15-/m0/s1
log P (octanol-water)	0.54
Henry's Law Constant	1.58E-26 atm-m <sup>3</sup> /mole
Vapor Pressure	1.14E-16 mm Hg
Water solubility	320 mg/L
Atmospheric OH Rate Constant	3.12E-10 cm <sup>3</sup> /molecule-sec



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