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## Typical Product Specifications & Properties

# 1-methylbarbituric acid

CAS Number: : 2565-47-1

Specifications	Limits
Molecular weight	142.11
EINECS	219-894-0
SMILES	<chem>O=C1NC(=O)N(C)C(=O)C1</chem>
InChI	DCGGMHIZEAHUJL-UHFFFAOYSA-N
InChIKey	1S/C5H6N2O3/c1-7-4(9)2-3(8)6-5(7)10/h2H2,1H3,(H,6,8,10)
log P (octanol-water)	-0.85
Atmospheric OH Rate Constant	3.08E-12 cm <sup>3</sup> /molecule-sec
Water solubility	4.37E+05 mg/L
Henry's Law Constant	2.55E-13 atm-m <sup>3</sup> /mole
pKa Dissociation Constant	4.35
Vapor Pressure	9.45E-09 mm Hg



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