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Typical Product Specifications & Properties

Ciglitazone

CAS Number: : 74772-77-3

Specifications	Limits
Molecular weight	333.45
SMILES	<chem>CC1(CCCCC1)COc2ccc(cc2)CC3C(=O)NC(=O)S3</chem>
InChI	YZFWTZACSRHJQD-UHFFFAOYSA-N
InChIKey	1S/C18H23NO3S/c1-18(9-3-2-4-10-18)12-22-14-7-5-13(6-8-14)11-15-16(20)19-17(21)23-15/h5-8,15H,2-4,9-12H2,1H3,(H,19,20,21)
Vapor Pressure	1.71E-12 mm Hg
Water solubility	3.620 mg/L
Henry's Law Constant	2.02E-08 atm-m ³ /mole
log P (octanol-water)	4
Atmospheric OH Rate Constant	8.10E-11 cm ³ /molecule-sec



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