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Typical Product Specifications & Properties

Thioxanthine

CAS Number: : 261-31-4

Specifications	Limits
Molecular weight	198.28
EINECS	205-972-1
SMILES	<chem>c1ccc2c(c1)Cc3ccccc3S2</chem>
InChI	1S/C13H10S/c1-3-7-12-10(5-1)9-11-6-2-4-8-13(11)14-12/h1-8H,9H2
InChIKey	PQJUJGAVDBINPI-UHFFFAOYSA-N
Boiling Point	341 ° C
log P (octanol-water)	4.550
Atmospheric OH Rate Constant	3.16E-11 cm3/molecule-sec
Melting Point	128.5 ° C



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