

Purine, 6-benzylthio-

Other names: 6-[(phenylmethyl)thio]-1H-purine.

InChI: InChI=1S/C12H10N4S/c1-2-4-9(5-3-1)6-17-12-10-11(14-7-13-10)15-8-16-12/h1-5,7-8H,6H2,(H,13,14,15,16)

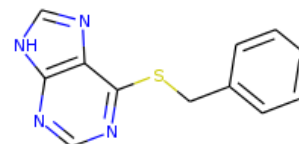
InChI Key: ULIQGBPQLPCTAJ-UHFFFAOYSA-N

Formula: C12H10N4S

SMILES: c1nc2c(ncnc2SCc2ccccc2)[nH]1

Molecular Weight: 242.30

CAS: 724-34-5



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	2.65		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H10N4S/c1-2-4-9\(5-3-1\)6-17-12-10-11\(14-7-13-10\)15-8-16-12/h1-5,7-8H,6H2,\(H,13,14,15,16\)](http://webbook.nist.gov/cgi/inchi/InChI=1S/C12H10N4S/c1-2-4-9(5-3-1)6-17-12-10-11(14-7-13-10)15-8-16-12/h1-5,7-8H,6H2,(H,13,14,15,16))

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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