Purine, 2,6-bis(benzylthio)-

Inchi: InChI=1S/C19H16N4S2/c1-3-7-14(8-4-1)11-24-18-16-17(21-13-20-16)22-19(23-18)25-12
InchiKey: UEWBQZTVHSBYIA-UHFFFAOYSA-N
Formula: C19H16N4S2
SMILES: c1ccc(CSc2nc(SCc3ccccc3)c3[nH]cnc3n2)cc1
Mol. weight [g/mol]: 364.49
CAS: 5441-77-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.50		Crippen Method
logp	4.456		Crippen Method
mcvol	264.750	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5441770&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume