

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

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<https://www.chemeo.com/cid/50-611-7/Purine-2-6-bis-benzylthio.pdf>

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