

Purine, 6-(o-chlorobenzyl thio)-

Inchi:	InChI=1S/C12H9ClN4S/c13-9-4-2-1-3-8(9)5-18-12-10-11(15-6-14-10)16-7-17-12/h1-4,6-
InchiKey:	ZITSATWAZDKOBF-UHFFFAOYSA-N
Formula:	C12H9ClN4S
SMILES:	Clc1ccccc1CSc1ncnc2nc[nH]c12
Mol. weight [g/mol]:	276.75
CAS:	5069-68-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.33		Crippen Method
logp	2.817		Crippen Method
mcvol	185.770	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5069681&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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/69-260-7/Purine-6-o-chlorobenzyl-thio.pdf>

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