

# Purine, 6-benzylthio-

<b>Other names:</b>	6-[(phenylmethyl)thio]-1H-purine
<b>Inchi:</b>	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,6
<b>InchiKey:</b>	ULIQGBPQLPCTAJ-UHFFFAOYSA-N
<b>Formula:</b>	C12H10N4S
<b>SMILES:</b>	c1ccc(CSc2ncnc3[nH]cnc23)cc1
<b>Mol. weight [g/mol]:</b>	242.30
<b>CAS:</b>	724-34-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.65		Crippen Method
logp	2.163		Crippen Method
mcvol	173.530	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C724345&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C724345&amp;Units=SI</a>

## Legend

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

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