Purine, 6-[p-(beta-chloroethylthio)anilino]-

Inchi:	InChI=1S/C13H12ClN5S/c14-5-6-20-10-3-1-9(2-4-10)19-13-11-12(16-7-15-11)17-8-18-1
InchiKey:	XYUCKJLYJVLRIO-UHFFFAOYSA-N
Formula:	C13H12ClN5S
SMILES:	ClCCSc1ccc(Nc2ncnc3[nH]cnc23)cc1
Mol. weight [g/mol]:	305.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.91		Crippen Method
logp	2.946		Crippen Method
mcvol	209.840	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008279&Units=SI

Legend

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

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