

Pyrimidine, 6-amino-4-benzyl(cyano)amino-2-benzylthio-

Inchi:	InChI=1S/C19H17N5S/c20-14-24(12-15-7-3-1-4-8-15)18-11-17(21)22-19(23-18)25-13-16
InchiKey:	YBXNDSSAEPQPNE-UHFFFAOYSA-N
Formula:	C19H17N5S
SMILES:	N#CN(Cc1ccccc1)c1cc(N)nc(SCc2ccccc2)n1
Mol. weight [g/mol]:	347.44
CAS:	98322-50-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.87		Crippen Method
logp	3.839		Crippen Method
mcvol	264.940	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C98322500&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/30-093-5/Pyrimidine-6-amino-4-benzyl-cyano-amino-2-benzylthio.pdf>

Generated by Cheméo on 2024-05-01 04:37:09.496951746 +0000 UTC m=+16827478.417529057.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.