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/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=C98322500&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume