Formamide, n-benzyl-n-[3-benzyl-6-benzylamino-4-thioxo-5-py

Inchi: InChI=1S/C26H24N4OS/c31-20-30(18-23-14-8-3-9-15-23)24-25(27-16-21-10-4-1-5-11-2

InchiKey: ADTOXRFWEALTQE-UHFFFAOYSA-N

Formula: C26H24N4OS

SMILES: O=CN(Cc1ccccc1)c1c(NCc2ccccc2)ncn(Cc2ccccc2)c1=S

Mol. weight [g/mol]: 440.56

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.56		Crippen Method
logp	5.436		Crippen Method
mcvol	340.000	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=B6010445&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume