

N,n'-diacetyl-n,n'-bis-[5-benzylmercapto-1,3,4-thia

Inchi:	InChI=1S/C22H20N6O2S4/c1-15(29)27(19-23-25-21(33-19)31-13-17-9-5-3-6-10-17)28(1
InchiKey:	WYNIAFSGHVXTNN-UHFFFAOYSA-N
Formula:	C22H20N6O2S4
SMILES:	CC(=O)N(c1nnc(SCc2ccccc2)s1)N(C(C)=O)c1nnc(SCc2ccccc2)s1
Mol. weight [g/mol]:	528.69
CAS:	102599-00-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.76		Crippen Method
logp	5.295		Crippen Method
mcvol	362.820	ml/mol	McGowan Method

Sources

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=C102599008&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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