Triazolo[4,5-d]pyrimidine, 3h-v-,5-amino-7-benzylthio-3-ethyl-

Inchi:	InChI=1S/C13H14N6S/c1-2-19-11-10(17-18-19)12(16-13(14)15-11)20-8-9-6-4-3-5-7-9/h3
InchiKey:	WRUMIWLCVFKRPY-UHFFFAOYSA-N
Formula:	C13H14N6S
SMILES:	CCn1nnc2c(SCc3ccccc3)nc(=N)[nH]c21
Mol. weight [g/mol]:	286.36
CAS:	96229-34-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.90		Crippen Method
logp	1.464		Crippen Method
mcvol	207.580	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C96229344&Units=SI
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

Legend

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

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