

Purine-8(9h)-thione, 7,9-bis-(piperidinomethyl)-

Inchi: InChI=1S/C17H26N6S/c24-17-22(13-20-7-3-1-4-8-20)15-11-18-12-19-16(15)23(17)14-21
InchiKey: CLIBGAKCPFAFDU-UHFFFAOYSA-N
Formula: C17H26N6S
SMILES: S=c1n(CN2CCCCC2)c2cncnc2n1CN1CCCCC1
Mol. weight [g/mol]: 346.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.45		Crippen Method
logp	2.849		Crippen Method
mcvol	265.980	ml/mol	McGowan Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008727&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/40-895-4/Purine-8-9h-thione-7-9-bis-piperidinomethyl.pdf>

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