9H-purine-9-acetic acid, 6(1h)-thio-, ethyl ester

Inchi:	InChI=1S/C9H10N4O2S/c1-2-15-6(14)3-13-5-12-7-8(13)10-4-11-9(7)16/h4-5H,2-3H2,1H
InchiKey:	YQVQDSNMIOZFMF-UHFFFAOYSA-N
Formula:	C9H10N4O2S
SMILES:	CCOC(=O)Cn1cnc2c(=S)[nH]cnc21
Mol. weight [g/mol]:	238.27
CAS:	99179-04-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	0.570		Crippen Method
mcvol	162.460	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=C99179041&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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.chemeo.com/cid/50-735-0/9H-purine-9-acetic-acid-6-1h-thio-ethyl-ester.pdf
Generated by Cheméo on 2024-10-12 04:25:56.525867561 +0000 UTC m=+3288019.162836814.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.