

9H-purine, 6-[(2-mercaptoethyl)thio]-, s-acetate

Inchi:	InChI=1S/C9H10N4OS2/c1-6(14)15-2-3-16-9-7-8(11-4-10-7)12-5-13-9/h4-5H,2-3H2,1H3
InchiKey:	CIJAISDDQRVOBA-UHFFFAOYSA-N
Formula:	C9H10N4OS2
SMILES:	CC(=O)SCCSc1ncnc2[nH]cnc12
Mol. weight [g/mol]:	254.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	1.243		Crippen Method
mcvol	172.940	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008692&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/61-148-0/9H-purine-6-2-mercaptoethyl-thio-s-acetate.pdf>

Generated by Cheméo on 2024-04-23 07:39:39.320557948 +0000 UTC m=+16147228.241135261.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.