Ethanol, 2-[(6(1h)-oxo-9h-purin-2-yl)thio]-(keto form)

Inchi: InChI=1S/C7H8N4O2S/c12-1-2-14-7-10-5-4(6(13)11-7)8-3-9-5/h3,12H,1-2H2,(H2,8,9,10

InchiKey: GKFGYZUHWYZCSN-UHFFFAOYSA-N

Formula: C7H8N4O2S

SMILES: O=c1[nH]c(SCCO)nc2[nH]cnc12

Mol. weight [g/mol]: 212.23

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.09		Crippen Method
logp	-1.233		Crippen Method
mcvol	138.580	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6008728&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume