Hypoxanthine-9-acetic acid, ethyl ester

Inchi: InChI=1S/C9H10N4O3/c1-2-16-6(14)3-13-5-12-7-8(13)10-4-11-9(7)15/h4-5H,2-3H2,1H3
InchiKey: LBXKMPLUVKYWSY-UHFFFAOYSA-N
Formula: C9H10N4O3
SMILES: CCOC(=O)Cn1cnc2c(=O)[nH]cnc21
Mol. weight [g/mol]: 222.20
CAS: 55175-33-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.41		Crippen Method
logp	-0.799		Crippen Method
mcvol	151.980	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=C55175332&Units=SI

Legend

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