

Acetic acid, [3-(1,2,3,4-tetrahydro-2,4-dioxo-5-pyrimidinyl)ureido-ethyl ester

InChI: InChI=1S/C9H12N4O5/c1-2-18-6(14)4-11-8(16)12-5-3-10-9(17)13-7(5)15/h3H,2,4H2,1H3
InChIKey: GSANXYWHYMONNG-UHFFFAOYSA-N
Formula: C9H12N4O5
SMILES: CCOC(=O)CNC(=O)Nc1c[nH]c(=O)[nH]c1=O
Mol. weight [g/mol]: 256.22
CAS: 7154-16-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.76		Crippen Method
logp	-2.216		Crippen Method
mcvol	174.580	ml/mol	McGowan Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C7154167&Units=SI>

Legend

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

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