4(3H)-pteridinone, 2-amino-6-(diethoxymethyl)- (keto form)

Inchi: InChI=1S/C11H15N5O3/c1-3-18-10(19-4-2)6-5-13-8-7(14-6)9(17)16-11(12)15-8/h5,10H,
InchiKey: LMQKFSOPTKYUEY-UHFFFAOYSA-N
Formula: C11H15N5O3
SMILES: CCOC(OCC)c1cnc2nc(N)[nH]c(=O)c2n1
Mol. weight [g/mol]: 265.27
CAS: 4227-30-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.04		Crippen Method
logp	-0.115		Crippen Method
mcvol	190.140	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=C4227309&Units=SI

Legend

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