

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/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=C4227309&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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