Benzo[g]pteridine-2,4(3H,10H)-dione,3,6,10-trimet

Inchi: InChI=1S/C13H12N4O2/c1-7-5-4-6-8-9(7)14-10-11(16(8)2)15-13(19)17(3)12(10)18/h4-6
InchiKey: NDERALLBJQVMHZ-UHFFFAOYSA-N
Formula: C13H12N4O2
SMILES: Cc1cccc2c1nc1c(=O)n(C)c(=O)nc-1n2C
Mol. weight [g/mol]: 256.26
CAS: 70481-66-2

Physical Properties

Property code	Value	Unit	Source
ie	8.16	eV	NIST Webbook
log10ws	-6.72		Crippen Method
logp	0.440		Crippen Method
mcvol	183.010	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=C70481662&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.