Benzo[g]pyrido[2,3d]pyrimidin-2,4-dione,3,7,8,10-

Inchi: InChI=1S/C15H15N3O2/c1-8-5-10-7-11-13(16-15(20)18(4)14(11)19)17(3)12(10)6-9(8)2/h
InchiKey: QVDSFYSCDJBRMC-UHFFFAOYSA-N
Formula: C15H15N3O2
SMILES: Cc1cc2cc3c(=O)n(C)c(=O)nc-3n(C)c2cc1C
Mol. weight [g/mol]: 269.30
CAS: 70239-57-5

Physical Properties

Property code	Value	Unit	Source
ie	7.94	eV	NIST Webbook
log10ws	-7.43		Crippen Method
logp	1.354		Crippen Method
mcvol	201.210	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=C70239575&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.