1,3-Thiazine-6-one-4-ol, 2-(3,4-dimethoxyphenyl)-

Inchi: InChI=1S/C12H11NO4S/c1-16-8-4-3-7(5-9(8)17-2)12-13-10(14)6-11(15)18-12/h3-6,14H,
InchiKey: MEOXNXVRBHADBM-UHFFFAOYSA-N
Formula: C12H11NO4S
SMILES: COc1ccc(-c2nc(O)cc(=O)s2)cc1OC
Mol. weight [g/mol]: 265.29
CAS: 95642-51-6

Physical Properties

Property code	Value	Unit	Source
ie	8.28	eV	NIST Webbook
log10ws	-2.81		Crippen Method
logp	1.893		Crippen Method
mcvol	182.230	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C95642516&Units=SI
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

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.