1-Oxo-2-(3-phenylrhodanin-5-ylidene)-3-pyridiniu

Inchi: InChI=1S/C24H14N2O3S2/c27-20-16-11-5-6-12-17(16)21(28)19(25-13-7-2-8-14-25)18(2
InchiKey: NCCDAIUPZIASNQ-UHFFFAOYSA-N
Formula: C24H14N2O3S2
SMILES: O=C1C(=C2SC(=S)N(c3ccccc3)C2=O)C([n+]2ccccc2)=C([O-])c2ccccc21
Mol. weight [g/mol]: 442.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.62		Crippen Method
logp	3.175		Crippen Method
mcvol	304.790	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6004427&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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