Bicyclo[4.2.0]octa-1,3,5-triene-7,8-dione

Inchi: InChI=1S/C8H4O2/c9-7-5-3-1-2-4-6(5)8(7)10/h1-4H
InchiKey: NFYYUUJYMWILSY-UHFFFAOYSA-N
Formula: C8H4O2
SMILES: O=c1c(=O)c2ccccc12
Mol. weight [g/mol]: 132.12
CAS: 6383-11-5

Physical Properties

Property code	Value	Unit	Source
ie	9.23	eV	NIST Webbook
log10ws	-0.95		Crippen Method
logp	0.436		Crippen Method
mcvol	92.100	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=C6383115&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.