2H,5H-Pyrano[4,3-b]pyran-2,5-dione, 4,7-dimethyl-

Other names: 4,7-Dimethyl-2H,5H-pyrano-[4,3-b]-pyran-2,5-dione
Inchi: InChI=1S/C10H8O4/c1-5-3-8(11)14-7-4-6(2)13-10(12)9(5)7/h3-4H,1-2H3
InchiKey: CLRUUBUGHDOXCJ-UHFFFAOYSA-N
Formula: C10H8O4
SMILES: Cc1cc2oc(=O)cc(C)c2c(=O)o1
Mol. weight [g/mol]: 192.17
CAS: 1204-38-2

Physical Properties

Property code	Value	Unit	Source
chs	-4642.00 ± 29.00	kJ/mol	NIST Webbook
hfs	-436.00 ± 29.00	kJ/mol	NIST Webbook
log10ws	-10.54		Crippen Method
logp	1.363		Crippen Method
mcvol	132.020	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1204382&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

chs: Standard solid enthalpy of combustion
hfs: Solid phase enthalpy of formation at standard conditions
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume