2,4-Pentanedione, 1-(7-acetyl-4,6-dihydroxy-3,5-dimethyl-2-benzofur

Other names: Decarbousnic acid
1-(7-Acetyl-4,6-dihydroxy-3,5-dimethylbenzofuran-2-yl)pentane-2,4-dione
Inchi: InChI=1S/C17H18O6/c1-7(18)5-11(20)6-12-8(2)13-15(21)9(3)16(22)14(10(4)19)17(13)23
InchiKey: BLYIQXWINBIBSV-UHFFFAOYSA-N
Formula: C17H18O6
SMILES: CC(=O)CC(=O)Cc1oc2c(C(C)=O)c(O)c(C)c(O)c2c1C
Mol. weight [g/mol]: 318.32
CAS: 21402-79-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.34		Crippen Method
logp	2.754		Crippen Method
mcvol	233.790	ml/mol	McGowan Method
rinpol	2679.10		NIST Webbook
rinpol	2679.10		NIST Webbook

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=C21402799&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices