Cyclopenta[c]pyran-7-carboxaldehyde, 4-[(acetyloxy)methyl]-

Other names: Cyclopenta[c]pyran-7-carboxaldehyde, 4-(hydroxymethyl)-, acetate
Baldrinal
4-(Hydroxymethyl)cyclopenta(c)pyran-7-carboxaldehyde acetate

Inchi: InChI=1S/C12H10O4/c1-8(14)16-6-10-5-15-7-12-9(4-13)2-3-11(10)12/h2-5,7H,6H2,1H3

InchiKey: QIUOVIRIFZOCLL-UHFFFAOYSA-N

Formula: C12H10O4

SMILES: CC(=O)OCc1cocc2c(C=O)ccc1-2

Mol. weight [g/mol]: 218.21

CAS: 18234-46-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.04		Crippen Method
logp	2.260		Crippen Method
mcvol	155.900	ml/mol	McGowan Method
rinpol	1911.90		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18234463&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

rinpol: Non-polar retention indices