

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

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