

2H-Pyran-5-carboxylic acid, 4,6-dimethyl-2-oxo-, ethyl ester

Other names:	Ethyl isodehydroacetate Ethyl 4,6-dimethyl-5-coumalate Ethyl 4,6-dimethyl-2-oxo-2H-pyran-5-carboxylate Ethyl 4,6-dimethyl-2-pyrone-5-carboxylate
Inchi:	InChI=1S/C10H12O4/c1-4-13-10(12)9-6(2)5-8(11)14-7(9)3/h5H,4H2,1-3H3
InchiKey:	FBPWNVQUVXSXKS-UHFFFAOYSA-N
Formula:	C10H12O4
SMILES:	CCOC(=O)c1c(C)cc(=O)oc1C
Mol. weight [g/mol]:	196.20
CAS:	3385-34-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.24		Crippen Method
logp	1.433		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
tb	565.70	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	410.00 ± 3.00	K	0.05	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C3385340&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure

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