2-Furoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C8H7ClO3/c9-4-2-6-12-8(10)7-3-1-5-11-7/h1-5H,6H2/b4-2+
InchiKey: IXYKCWJROBXCPM-DUXPYHPUSA-N
Formula: C8H7ClO3
SMILES: O=C(OCC=CCl)c1ccco1
Mol. weight [g/mol]: 186.59

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.79		Crippen Method
logp	2.189		Crippen Method
mcvol	125.370	ml/mol	McGowan Method
rinpol	1332.00		NIST Webbook
rinpol	1332.00		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=U299242&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

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