3,4-Furandicarboxylic acid, diethyl ester

Other names:	Diethyl 3,4-furandicarboxylate
	diethyl furan-3,4-dicarboxylate
Inchi:	InChI=1S/C10H12O5/c1-3-14-9(11)7-5-13-6-8(7)10(12)15-4-2/h5-6H,3-4H2,1-2H3
InchiKey:	ZODFWNHYQARJLC-UHFFFAOYSA-N
Formula:	C10H12O5
SMILES:	CCOC(=O)c1cocc1C(=O)OCC
Mol. weight [g/mol]:	212.20
CAS:	30614-77-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.53		Crippen Method
logp	1.633		Crippen Method
mcvol	153.050	ml/mol	McGowan Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	428.20	K	1.70	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=C30614778&Units=SI

Legend

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