

2,5-Pyrazinedicarboxylic acid, dimethyl ester

Inchi:	InChI=1S/C8H8N2O4/c1-13-7(11)5-3-10-6(4-9-5)8(12)14-2/h3-4H,1-2H3
InchiKey:	DQGTXXDDKDMEHB-UHFFFAOYSA-N
Formula:	C8H8N2O4
SMILES:	COC(=O)c1cnc(C(=O)OC)cn1
Mol. weight [g/mol]:	196.16
CAS:	13051-89-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.49		Crippen Method
logp	0.050		Crippen Method
mcvol	134.660	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13051893&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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