

α,α'-Dimethylmuconic acid

Other names:	2,5-Dimethyl-2,4-hexadienedioic acid
Inchi:	InChI=1S/C8H10O4/c1-5(7(9)10)3-4-6(2)8(11)12/h3-4H,1-2H3,(H,9,10)(H,11,12)/b5-3+,6
InchiKey:	HVMNFKUBOVSQCO-GGWOSOGESA-N
Formula:	C8H10O4
SMILES:	CC(=CC=C(C)C([O])=O)C([O])=O
Mol. weight [g/mol]:	170.16
CAS:	20514-41-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.21		Crippen Method
logp	0.793		Crippen Method
mcvol	125.560	ml/mol	McGowan Method

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=C20514414&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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