

Malonic acid, TMS, secondary peak (unknown)

Inchi: InChI=1S/C6H12O4Si/c1-11(2,3)10-6(9)4-5(7)8/h4H2,1-3H3,(H,7,8)
InchiKey: YOPGTPLFLDXOQM-UHFFFAOYSA-N
Formula: C6H12O4Si
SMILES: C[Si](C)(C)OC(=O)CC(=O)O
Mol. weight [g/mol]: 176.24

Physical Properties

Property code	Value	Unit	Source
log10ws	1.65		Crippen Method
logp	0.839		Crippen Method
rinpol	1432.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R95000&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/31-898-1/Malonic-acid-TMS-secondary-peak-unknown.pdf>

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