

Methyl diazoacetate

Inchi: InChI=1S/C3H4N2O2/c1-7-3(6)2-5-4/h2H,1H3
InchiKey: MIVRMHJOEYRXQB-UHFFFAOYSA-N
Formula: C3H4N2O2
SMILES: COC(=O)C=[N+]=[N-]
Mol. weight [g/mol]: 100.08

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.58		Crippen Method
logp	-0.540		Crippen Method
mcvol	71.930	ml/mol	McGowan Method
rinpol	757.00		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	757.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=R633106&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

Latest version available from:

<https://www.chemeo.com/cid/116-609-7/Methyl-diazoacetate.pdf>

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