

# Isopropyl diazoacetate

**Inchi:** InChI=1S/C5H8N2O2/c1-4(2)9-5(8)3-7-6/h3-4H,1-2H3  
**InchiKey:** FNXAUCKBTPCLJL-UHFFFAOYSA-N  
**Formula:** C5H8N2O2  
**SMILES:** CC(C)OC(=O)C=[N+]=[N-]  
**Mol. weight [g/mol]:** 128.13

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.53		Crippen Method
logp	0.239		Crippen Method
mcvol	100.110	ml/mol	McGowan Method
rinpol	875.00		NIST Webbook
rinpol	902.00		NIST Webbook
rinpol	875.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=R633097&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

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