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/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=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

Latest version available from:
https://www.chemeo.com/cid/123-886-2/Isopropyl-diazoacetate.pdf

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