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