

2-Diazo-6-oxo-2,6-dihydroazulene-1,3-dicarboxylic acid, diethyl ester

InChI: InChI=1S/C16H14N2O5/c1-3-22-15(20)12-10-7-5-9(19)6-8-11(10)13(14(12)18-17)16(21)2
InChIKey: MXIFE0YDIGRKLQ-UHFFFAOYSA-N

Formula: C16H14N2O5
SMILES: CCOC(=O)C1=c2ccc(=O)ccc2=C(C(=O)OCC)C1=[N+]=[N-]
Mol. weight [g/mol]: 314.29
CAS: 53535-43-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.54		Crippen Method
logp	-0.841		Crippen Method
mcvol	225.190	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C53535436&Units=SI>
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>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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