

9-Diazo-4,5-methylene-10-oxophenanthrene

Inchi:	InChI=1S/C15H8N2O/c16-17-14-10-5-1-3-8-7-9-4-2-6-11(15(14)18)13(9)12(8)10/h1-6H,7
InchiKey:	YOLUZYYSQYYNX-UHFFFAOYSA-N
Formula:	C15H8N2O
SMILES:	[N-]=[N+]=C1C(=O)c2cccc3c2-c2c(cccc21)C3
Mol. weight [g/mol]:	232.24
CAS:	24153-37-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.68		Crippen Method
logp	2.473		Crippen Method
mcvol	165.900	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C24153375&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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