

cis-Nitrosobenzene dimer

Inchi:	InChI=1S/C12H10N2O2/c15-13(11-7-3-1-4-8-11)14(16)12-9-5-2-6-10-12/h1-10H/b14-13
InchiKey:	WHFNSVMCGRQIRC-YPKPFQOOSA-N
Formula:	C12H10N2O2
SMILES:	[O-][N+](c1ccccc1)=[N+][O-]c1ccccc1
Mol. weight [g/mol]:	214.22
CAS:	31077-80-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	3.123		Crippen Method
mcvol	159.820	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C31077802&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.chemeo.com/cid/70-121-9/cis-Nitrosobenzene-dimer.pdf>

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