

Bis(pentamethylphenyl)diazene, N,N'-dioxide

Inchi:	InChI=1S/C22H30N2O2/c1-11-13(3)17(7)21(18(8)14(11)4)23(25)24(26)22-19(9)15(5)12
InchiKey:	CQHBMGBXOHZXMFWCWDXBQESA-N
Formula:	C22H30N2O2
SMILES:	Cc1c(C)c(C)c([N+])([O-])=[N+](O-)]c2c(C)c(C)c(C)c(C)c2C)c(C)c1C
Mol. weight [g/mol]:	354.49
CAS:	84802-30-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.05		Crippen Method
logp	6.207		Crippen Method
mcvol	300.720	ml/mol	McGowan Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84802302&Units=SI

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/58-382-4/Bis-pentamethylphenyl-diazene-N-N-dioxide.pdf>

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