

4,4'-Dimethoxydiphenylnitrogen oxide

Inchi: InChI=1S/C14H14NO3/c1-17-13-7-3-11(4-8-13)15(16)12-5-9-14(18-2)10-6-12/h3-10H,1-
InchiKey: NJQKHLCLMSKSKD-UHFFFAOYSA-N
Formula: C14H14NO3
SMILES: COc1ccc(N([O])c2ccc(OC)cc2)cc1
Mol. weight [g/mol]: 244.27
CAS: 2643-00-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.88		Crippen Method
logp	3.187		Crippen Method
mccvol	186.040	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hsubt	100.70	kJ/mol	345.50	NIST Webbook
hsubt	100.70 ± 2.60	kJ/mol	328.00	NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2643007&Units=SI>
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>

Legend

hsubt: Enthalpy of sublimation at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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