

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
InchiKey: WHFNSVMCGRQIRC-UHFFFAOYSA-N
Formula: C12H10N2O2
SMILES: [O-][N+](c1ccccc1)=[N+](O)c1ccccc1
Mol. weight [g/mol]: 214.22
CAS: 35506-28-6

Physical Properties

Property code	Value	Unit	Source
chs	-6393.00 ± 2.00	kJ/mol	NIST Webbook
hf	328.00 ± 3.00	kJ/mol	NIST Webbook
hfs	241.00 ± 2.00	kJ/mol	NIST Webbook
hsub	87.00 ± 0.80	kJ/mol	NIST Webbook
log10ws	-3.29		Crippen Method
logp	3.123		Crippen Method
mcvol	159.820	ml/mol	McGowan Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C115626830&Units=SI>

Legend

chs: Standard solid enthalpy of combustion
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hsub: Enthalpy of sublimation at standard conditions
log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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