Benzenamine, N-[(4-methoxyphenyl)methylene]-, N-oxide

Other names: Nitrone, «alpha»-(p-methoxyphenyl)-N-phenyl-
«alpha»-(p-Methoxyphenyl)-N-phenylnitrone
«alpha»-4'-Methoxyphenyl N-phenylnitrone

Inchi: InChI=1S/C14H13NO2/c1-17-14-9-7-12(8-10-14)11-15(16)13-5-3-2-4-6-13/h2-11H,1H3

InchiKey: GIBHBSRKHBYUKU-UHFFFAOYSA-N

Formula: C14H13NO2

SMILES: COc1ccc(C=[N+]([O-])c2ccccc2)cc1

Mol. weight [g/mol]: 227.26

CAS: 3585-93-1

Physical Properties

Property code	Value	Unit	Source
chs	-7346.10 ± 1.20	kJ/mol	NIST Webbook
hf	109.70 ± 2.50	kJ/mol	NIST Webbook
hfs	-20.90 ± 2.20	kJ/mol	NIST Webbook
hsub	130.60 ± 1.20	kJ/mol	NIST Webbook
hsub	130.60 ± 1.20	kJ/mol	NIST Webbook
log10ws	-3.35		Crippen Method
logp	2.956		Crippen Method
mcvol	178.020	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=C3585931&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