2-Propanamine, 2-methyl-N-(phenylmethylene)-, N-oxide

Other names: N-tert-Butyl-«alpha»-phenylnitrone
N-t-Butyl-«alpha»-phenylnitrone
Phenyl N-tert-butylnitrone
N-benzyliden-tert-butylamine N-ether

Inchi: InChI=1S/C11H15NO/c1-11(2,3)12(13)9-10-7-5-4-6-8-10/h4-9H,1-3H3

InchiKey: IYSYLWYGCWTJSG-UHFFFAOYSA-N

Formula: C11H15NO

SMILES: CC(C)(C)[N+]([O-])=Cc1ccccc1

Mol. weight [g/mol]: 177.24

CAS: 3376-24-7

Physical Properties

Property code	Value	Unit	Source
chs	-6416.40 ± 1.10	kJ/mol	NIST Webbook
hf	30.90 ± 2.00	kJ/mol	NIST Webbook
hfs	-55.90 ± 1.80	kJ/mol	NIST Webbook
hsub	86.80 ± 0.90	kJ/mol	NIST Webbook
hsub	86.80 ± 0.90	kJ/mol	NIST Webbook
ie	7.69	eV	NIST Webbook
log10ws	-2.80		Crippen Method
logp	2.414		Crippen Method
mcvol	153.640	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3376247&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

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