

# 4-Isopropylbenzylidene t-butylamine N-oxide

**Inchi:** InChI=1S/C14H21NO/c1-11(2)13-8-6-12(7-9-13)10-15(16)14(3,4)5/h6-11H,1-5H3/b15-10  
**InchiKey:** NWCMTMPBYSGWMZ-GDNBJRDFSAN  
**Formula:** C14H21NO  
**SMILES:** CC(C)c1ccc(C=[N+])([O-])C(C)(C)C)cc1  
**Mol. weight [g/mol]:** 219.32  
**CAS:** 121678-88-4

## Physical Properties

Property code	Value	Unit	Source
chs	-8357.70 ± 1.80	kJ/mol	NIST Webbook
hf	-50.90 ± 4.90	kJ/mol	NIST Webbook
hfs	-152.70 ± 2.60	kJ/mol	NIST Webbook
hsub	101.80 ± 4.10	kJ/mol	NIST Webbook
hsub	101.80 ± 4.10	kJ/mol	NIST Webbook
log10ws	-3.98		Crippen Method
logp	3.538		Crippen Method
mcvol	195.910	ml/mol	McGowan Method

## Sources

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C121678884&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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