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-GDNBJRDFSA-N
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
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/ci990307l

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