4-t-Butylpyridine-N-oxide

Other names: Pyridine,4-(1,1-dimethylethyl)-,1-oxide
4-t-Butylpyridine-N-oxide
Inchi: InChI=1S/C9H13NO/c1-9(2,3)8-4-6-10(11)7-5-8/h4-7H,1-3H3
InchiKey: CMFQXPIZAKBRCG-UHFFFAOYSA-N
Formula: C9H13NO
SMILES: CC(C)(C)c1cc[n+]([O-])cc1
Mol. weight [g/mol]: 151.21

Physical Properties

Property code	Value	Unit	Source
af	0.3647		Cheméo Relay (1.0)
hf	27.70	kJ/mol	Cheméo Relay (1.0)
hvap	70.75	kJ/mol	Cheméo Relay (1.0)
ie	7.80	eV	NIST Webbook
ie	8.00	eV	NIST Webbook
log10ws	-1.91		Cheméo Relay (1.0)
logp	1.617		Crippen Method
mcvol	129.760	ml/mol	McGowan Method
pc	3072.74	kPa	Cheméo Relay (1.0, beta)
tb	495.51	K	Cheméo Relay (1.0)
tc	706.97	K	Cheméo Relay (1.0)
tf	395.13	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23569177&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point