2-tert-Butylpyridine

Other names:	Pyridine, 2-(1,1-dimethylethyl)-
	2-t-Butylpyridine
	2-(t-C4H9)-Pyridine
Inchi:	InChI=1S/C9H13N/c1-9(2,3)8-6-4-5-7-10-8/h4-7H,1-3H3
InchiKey:	UUIMDJFBHNDZOW-UHFFFAOYSA-N
Formula:	C9H13N
SMILES:	CC(C)(C)c1ccccn1
Mol. weight [g/mol]:	135.21
CAS:	5944-41-2

Physical Properties

Property code	Value	Unit	Source
affp	961.70	kJ/mol	NIST Webbook
basg	929.80	kJ/mol	NIST Webbook
log10ws	-2.55		Crippen Method
logp	2.379		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
tf	240.35 ± 0.30	K	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	442.20	K	99.10	NIST Webbook

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=C5944412&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point