

2,6-Di-tert-butylpyridine

Other names:	2,6-(t-C4H9)2-pyridine 2,6-di-t-Butylpyridine Pyridine, 2,6-di-tert-butyl-
Inchi:	InChI=1S/C13H21N/c1-12(2,3)10-8-7-9-11(14-10)13(4,5)6/h7-9H,1-6H3
InchiKey:	UWKQJZCTQGMHKD-UHFFFAOYSA-N
Formula:	C13H21N
SMILES:	CC(C)(C)c1cccc(C(C)(C)C)n1
Mol. weight [g/mol]:	191.32

Physical Properties

Property code	Value	Unit	Source
affp	982.90	kJ/mol	NIST Webbook
basg	951.00	kJ/mol	NIST Webbook
hvap	56.60 ± 1.20	kJ/mol	NIST Webbook
ie	8.56	eV	Cheméo Relay (1.0)
logp	3.677		Crippen Method
mcvol	180.250	ml/mol	McGowan Method
tf	320.62	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hvapt	56.60	kJ/mol	298.15	Thermochemical Study of Three Hindered Pyridine Derivatives

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.70	K	3.10	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Experimental and statistical mechanical studies of heats of dilution of amides in pyridine derivatives	https://www.doi.org/10.1016/j.fluid.2006.07.004
Thermodynamic study of the hydrogen bonding energies of	https://www.doi.org/10.1021/je800155q
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C585488&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point

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