

2-(t-C4H9)-pyridine

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

Physical Properties

Property code	Value	Unit	Source
af	0.3251		Cheméo Relay (1.0)
gf	185.77	kJ/mol	Cheméo Relay (1.0, beta)
hf	17.70	kJ/mol	Cheméo Relay (1.0)
hvap	47.82	kJ/mol	Cheméo Relay (1.0)
ie	9.02	eV	Cheméo Relay (1.0)
log10ws	-1.29		Cheméo Relay (1.0)
logp	2.379		Crippen Method
mcvol	123.890	ml/mol	McGowan Method
pc	3129.03	kPa	Cheméo Relay (1.0, beta)
tb	442.19	K	Cheméo Relay (1.0)
tc	661.17	K	Cheméo Relay (1.0)
tf	231.29	K	Cheméo Relay (1.0)
vc	0.451	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5944412&Units=SI>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
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
vc:	Critical Volume

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