Pyridine, 2,4,6-trimethyl-

Other names:	2,4,6-COLLIDINE
	2,4,6-Kollidin
	2,4,6-Trimethylpyridine
	NSC 460
	S-COLLIDINE
	gamma-Collidine
	sym-Collidine
	«alpha»,«gamma»,«alpha»'-Collidine
	«gamma»-Collidine
	Â«alphaÂ»,Â«gammaÂ»,Â«alphaÂ»'-Collidine
	Â«gammaÂ»-Collidine
Inchi:	InChI=1S/C8H11N/c1-6-4-7(2)9-8(3)5-6/h4-5H,1-3H3
InchiKey:	BWZVCCNYKMEVEX-UHFFFAOYSA-N
Formula:	C8H11N
SMILES:	Cc1cc(C)nc(C)c1
Mol. weight [g/mol]:	121.18
CAS:	108-75-8

Physical Properties

Property code	Value	Unit	Source
af	0.4130		KDB
chl	-4689.10 ± 2.00	kJ/mol	NIST Webbook
hfl	-31.00 ± 2.30	kJ/mol	NIST Webbook
hvap	50.40 ± 2.90	kJ/mol	NIST Webbook
hvap	50.30 ± 0.20	kJ/mol	NIST Webbook
hvap	50.20	kJ/mol	NIST Webbook
ie	8.90 ± 0.10	eV	NIST Webbook
log10ws	-2.66		Crippen Method
logp	2.007		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3200.00	kPa	KDB
rinpol	976.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	985.00		NIST Webbook

rinpol	982.00		NIST Webbook
rinpol	972.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	986.60		NIST Webbook
rinpol	986.60		NIST Webbook
rinpol	977.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	996.00		NIST Webbook
rinpol	999.00		NIST Webbook
rinpol	976.50		NIST Webbook
rinpol	1004.00		NIST Webbook
rinpol	158.66		NIST Webbook
rinpol	1012.00		NIST Webbook
rinpol	987.00		NIST Webbook
ripol	1368.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1410.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1397.00		NIST Webbook
ripol	1405.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1362.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1378.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1358.00		NIST Webbook
ripol	1371.00		NIST Webbook
ripol	1398.00		NIST Webbook
ripol	1372.00		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1365.00		NIST Webbook
ripol	1355.00		NIST Webbook
ripol	1375.00		NIST Webbook
ripol	1402.00		NIST Webbook
tb	443.50	K	KDB
tc	645.00	K	KDB
tf	228.95 ± 0.05	K	NIST Webbook
tf	229.00	K	KDB
tf	228.15 ± 1.00	K	NIST Webbook
tf	228.69 ± 0.10	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpl	215.10	J/mol×K	300.60	NIST Webbook
hfust	9.54	kJ/mol	228.96	NIST Webbook
hfust	9.54	kJ/mol	229.00	NIST Webbook
hfust	9.54	kJ/mol	229.00	NIST Webbook
hvapt	46.50	kJ/mol	363.50	NIST Webbook
hvapt	51.20	kJ/mol	371.00	NIST Webbook
hvapt	48.30	kJ/mol	328.00	NIST Webbook
hvapt	47.20	kJ/mol	343.00	NIST Webbook
hvapt	45.50	kJ/mol	368.00	NIST Webbook
rhol	702.86	kg/m3	293.10	KDB
rhol	928.45	kg/m3	276.15	Volumetric Properties of Binary Mixtures of 2,4,6-Trimethylpyridine with 1,2-Ethanediol, Methanol, and Water, and the Association Energies of the O-H***N Bonded Complexes
rhol	927.61	kg/m3	277.15	Volumetric Properties of Binary Mixtures of 2,4,6-Trimethylpyridine with 1,2-Ethanediol, Methanol, and Water, and the Association Energies of the O-H***N Bonded Complexes
rhol	922.54	kg/m3	283.15	Volumetric Properties of Binary Mixtures of 2,4,6-Trimethylpyridine with 1,2-Ethanediol, Methanol, and Water, and the Association Energies of the O-H***N Bonded Complexes

rhol	918.32	kg/m3	288.15	Volumetric Properties of Binary Mixtures of 2,4,6-Trimethylpyridine with 1,2-Ethanediol, Methanol, and Water, and the Association Energies of the O-H***N Bonded Complexes
rhol	914.08	kg/m3	293.14	Volumetric Properties of Binary Mixtures of 2,4,6-Trimethylpyridine with 1,2-Ethanediol, Methanol, and Water, and the Association Energies of the O-H***N Bonded Complexes
rhol	909.84	kg/m3	298.15	Volumetric Properties of Binary Mixtures of 2,4,6-Trimethylpyridine with 1,2-Ethanediol, Methanol, and Water, and the Association Energies of the O-H***N Bonded Complexes
rhol	905.58	kg/m3	303.15	Volumetric Properties of Binary Mixtures of 2,4,6-Trimethylpyridine with 1,2-Ethanediol, Methanol, and Water, and the Association Energies of the O-H***N Bonded Complexes
rhol	901.31	kg/m3	308.15	Volumetric Properties of Binary Mixtures of 2,4,6-Trimethylpyridine with 1,2-Ethanediol, Methanol, and Water, and the Association Energies of the O-H***N Bonded Complexes

rhol	897.03	kg/m3	313.15	Volumetric Properties of Binary Mixtures of 2,4,6-Trimethylpyridine with 1,2-Ethanediol, Methanol, and Water, and the Association Energies of the O-H***N Bonded Complexes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.46994e+01
Coeff. B	-3.82577e+03
Coeff. C	-6.44990e+01
Temperature range (K), min.	329.96
Temperature range (K), max.	472.02

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Volumetric Properties of Binary Mixtures of 2,4,6-Trimethylpyridine with 1,2-Ethanediol, Methanol, and Water, and the Association Energies of the O-H*N Bonded Complexes:**	https://www.doi.org/10.1007/s10765-011-1149-x
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1361.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C108758&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

af:	Acentric Factor
chl:	Standard liquid enthalpy of combustion

cpl:	Liquid phase heat capacity
hfl:	Liquid phase enthalpy of formation at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point