Pyridine, 2,3,4-trimethyl-

Other names: Pyridine, 2,3,4-trimethyl-
Inchi: InChI=1S/C8H11N/c1-6-4-5-9-8(3)7(6)2/h4-5H,1-3H3
InchiKey: HOPRXXXSABQWAV-UHFFFAOYSA-N
Formula: C8H11N
SMILES: Cc1ccnc(C)c1C
Mol. weight [g/mol]: 121.18

Physical Properties

Property code	Value	Unit	Source
af	0.3570		Cheméo Relay (1.0)
hf	36.47	kJ/mol	Cheméo Relay (1.0)
hvap	50.26	kJ/mol	Cheméo Relay (1.0)
ie	8.82	eV	Cheméo Relay (1.0)
log10ws	-0.42		Cheméo Relay (1.0)
logp	2.007		Crippen Method
mcvol	109.800	ml/mol	McGowan Method
pc	3938.60	kPa	Cheméo Relay (1.0, beta)
rinpol	1099.00		NIST Webbook
rinpol	1084.00		NIST Webbook
ripol	1541.00		NIST Webbook
ripol	1541.00		NIST Webbook
tb	459.25	K	Cheméo Relay (1.0)
tc	681.40	K	Cheméo Relay (1.0)
tf	283.05	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2233296&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
Cheméo Relay (1.0):

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point