

4-Pyridineethanol

Inchi:	InChI=1S/C7H9NO/c9-6-3-7-1-4-8-5-2-7/h1-2,4-5,9H,3,6H2
InchiKey:	DWPYQDGDWBKJQL-UHFFFAOYSA-N
Formula:	C7H9NO
SMILES:	OCCc1ccncc1
Mol. weight [g/mol]:	123.15
CAS:	5344-27-4

Physical Properties

Property code	Value	Unit	Source
af	0.6305		Cheméo Relay (1.0)
hf	-83.14	kJ/mol	Cheméo Relay (1.0)
hvap	71.43	kJ/mol	Cheméo Relay (1.0)
ie	9.59	eV	Cheméo Relay (1.0)
log10ws	0.69		Cheméo Relay (1.0)
logp	0.616		Crippen Method
mvol	101.580	ml/mol	McGowan Method
pc	4573.40	kPa	Cheméo Relay (1.0, beta)
tb	524.20	K	Cheméo Relay (1.0)
tc	773.55	K	Cheméo Relay (1.0)
tf	282.15	K	Jean-Claude Bradley Open Melting Point Dataset (2014, CC0)

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
Jean-Claude Bradley Open Melting Point Dataset (2014, CC0):	https://figshare.com/articles/Jean_Claude_Bradley_Open_Melting_Point_Dataset/1031637
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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