2-PYRIDINEPROPANOL

Other names:	2-Pyridinepropanol
	2-Propanol pyridine
	2-Pyridylpropanol
	3-(2-Pyridyl)propanol
	2-(3-Hydroxypropyl)pyridine
	3-(2-Pyridyl)propan-1-ol
Inchi:	InChI=1S/C8H11NO/c10-7-3-5-8-4-1-2-6-9-8/h1-2,4,6,10H,3,5,7H2
InchiKey:	FVZXYJDGVYLMDB-UHFFFAOYSA-N
Formula:	C8H11NO
SMILES:	OCCCc1ccccn1
Mol. weight [g/mol]:	137.18

Physical Properties

Property code	Value	Unit	Source
af	0.6638		Cheméo Relay (1.0)
hvap	79.57	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	0.52		Cheméo Relay (1.0)
logp	1.006		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
pc	4206.00	kPa	Cheméo Relay (1.0, beta)
rinpol	1223.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1276.00		NIST Webbook
tb	525.08	K	Cheméo Relay (1.0)
tc	770.86	K	Cheméo Relay (1.0)
tf	276.49	K	Cheméo Relay (1.0)

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	374.20	K	0.30	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2859689&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):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point