

3-(2-Pyridyl)-1-propanol

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:	OCCc1ccccc1
Mol. weight [g/mol]:	137.18
CAS:	2859-68-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.72		Crippen Method
logp	1.006		Crippen Method
mcvol	115.670	ml/mol	McGowan Method
rinpol	1276.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1276.00		NIST Webbook

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

Crippen Method:

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

McGowan Method:

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tbrp:	Boiling point at reduced pressure

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