

DIPHENYL(2-PYRIDYL)METHANOL

Other names:	Diphenyl-(2-pyridyl)carbinol
Inchi:	InChI=1S/C18H15NO/c20-18(15-9-3-1-4-10-15,16-11-5-2-6-12-16)17-13-7-8-14-19-17/h
InchiKey:	IBNTYLTYDKBLRC-UHFFFAOYSA-N
Formula:	C18H15NO
SMILES:	OC(c1ccccc1)(c1ccccc1)c1cccn1
Mol. weight [g/mol]:	261.32

Physical Properties

Property code	Value	Unit	Source
hvap	93.80	kJ/mol	Cheméo Relay (1.0)
ie	8.75	eV	Cheméo Relay (1.0)
log10ws	-2.75		Cheméo Relay (1.0)
logp	3.366		Crippen Method
mcvol	209.050	ml/mol	McGowan Method
rinpol	2161.00		NIST Webbook
rinpol	2161.00		NIST Webbook
ripol	3114.00		NIST Webbook
ripol	3114.00		NIST Webbook
tb	622.14	K	Cheméo Relay (1.0)
tf	371.08	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C19490905&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

Legend

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

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