

1-Hydroxy-2-(2,4,6-trimethyl) naphthalide

Inchi:	lnChI=1S/C20H19NO2/c1-12-10-13(2)18(14(3)11-12)21-20(23)17-9-8-15-6-4-5-7-16(15)
InchiKey:	BJTNZOWFBLAJSD-UHFFFAOYSA-N
Formula:	C20H19NO2
SMILES:	Cc1cc(C)c(N=C(O)c2ccc3cccc3c2O)c(C)c1
Mol. weight [g/mol]:	305.37
CAS:	110150-56-6

Physical Properties

Property code	Value	Unit	Source
hf	-94.99	kJ/mol	Joback Method
hvap	102.04	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	5.107		Crippen Method
mcvol	243.100	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
tb	998.62	K	Joback Method
tc	1246.40	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110150566&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
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

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