

Benzoic acid, p-[(6-hydroxy-3,4-xylyl)azo]-

Inchi:	InChI=1S/C15H14N2O3/c1-9-7-13(14(18)8-10(9)2)17-16-12-5-3-11(4-6-12)15(19)20/h3-8,14,16,19,20
InchiKey:	IRPMNRQJHGUWHK-WUKNDPDISA-N
Formula:	C15H14N2O3
SMILES:	Cc1cc(O)c(N=Nc2ccc(C(=O)O)cc2)cc1C
Mol. weight [g/mol]:	270.28
CAS:	3810-51-3

Physical Properties

Property code	Value	Unit	Source
hf	-309.18	kJ/mol	Joback Method
hvap	98.63	kJ/mol	Joback Method
log10ws	-4.07		Crippen Method
logp	4.123		Crippen Method
mcvol	203.660	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
tb	986.77	K	Joback Method
tc	1234.50	K	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3810513&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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