2-Hydroxybenzaldehyde O-pentafluorophenylmethyl-oxime

Other names: 2-Hydroxybenzaldehyde O-2,3,4,5,6-PFBHA-oxime
Salicylic aldehyde, PFBO # 1

Inchi: InChI=1S/C14H8F5NO2/c15-10-8(11(16)13(18)14(19)12(10)17)6-22-20-5-7-3-1-2-4-9(7)

InchiKey: BWNAPEPFRCHYRY-UHFFFAOYSA-N

Formula: C14H8F5NO2

SMILES: Oc1ccccc1C=NOCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 317.21

Physical Properties

Property code	Value	Unit	Source
hf	-1124.44	kJ/mol	Joback Method
hvap	69.27	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.638		Crippen Method
mcvol	186.870	ml/mol	McGowan Method
pc	2117.78	kPa	Joback Method
rinpol	1845.00		NIST Webbook
rinpol	1845.00		NIST Webbook
ripol	2675.00		NIST Webbook
ripol	2675.00		NIST Webbook
tb	774.05	K	Joback Method
tc	987.57	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U372209&Units=SI

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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature