

benzaldehyde oxime, 2-hydroxy, 5-ethyl-

Inchi: InChI=1S/C9H11NO2/c1-2-7-3-4-9(11)8(5-7)6-10-12/h3-6,11-12H,2H2,1H3
InchiKey: ZKNUMEVCCQQDQKY-UHFFFAOYSA-N
Formula: C9H11NO2
SMILES: CCc1ccc(O)c(C=NO)c1
Mol. weight [g/mol]: 165.19

Physical Properties

Property code	Value	Unit	Source
hf	-251.35	kJ/mol	Joback Method
hvap	71.57	kJ/mol	Joback Method
log10ws	-1.13		Crippen Method
logp	1.763		Crippen Method
mcvol	131.330	ml/mol	McGowan Method
pc	3763.78	kPa	Joback Method
rinpol	1693.00		NIST Webbook
tb	686.46	K	Joback Method
tc	907.37	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R256987&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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