

benzaldehyde oxime, 2-hydroxy, 5-hexyl

Inchi: InChI=1S/C13H19NO2/c1-2-3-4-5-6-11-7-8-13(15)12(9-11)10-14-16/h7-10,15-16H,2-6H2
InchiKey: RDPQFZLMSKPPPZ-UHFFFAOYSA-N
Formula: C13H19NO2
SMILES: CCCCCC1CCC(O)c(C=NO)c1
Mol. weight [g/mol]: 221.30

Physical Properties

Property code	Value	Unit	Source
hf	-333.91	kJ/mol	Joback Method
hvap	80.48	kJ/mol	Joback Method
log10ws	-2.80		Crippen Method
logp	3.323		Crippen Method
mcvol	187.690	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	2031.00		NIST Webbook
tb	777.98	K	Joback Method
tc	987.36	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=R256992&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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