anti-phenylacetaldoxime

Inchi: InChI=1S/C8H9NO/c10-9-7-6-8-4-2-1-3-5-8/h1-5,7,10H,6H2
InchiKey: CXISHLWVCSLKOJ-UHFFFAOYSA-N
Formula: C8H9NO
SMILES: ON=CCc1ccccc1
Mol. weight [g/mol]: 135.16

Physical Properties

Property code	Value	Unit	Source
hf	-41.93	kJ/mol	Joback Method
hvap	55.67	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	1.689		Crippen Method
mcvol	111.370	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	1278.00		NIST Webbook
tb	577.98	K	Joback Method
tc	792.50	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R406692&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature