Phenylacetaldehyde, O-methyloxime, (E)

Inchi: InChI=1S/C9H11NO/c1-11-10-8-7-9-5-3-2-4-6-9/h2-6,8H,7H2,1H3/b10-8+
InchiKey: NICHQMGWWYWONX-CSKARUKUSA-N
Formula: C9H11NO
SMILES: CON=CCc1ccccc1
Mol. weight [g/mol]: 149.19

Physical Properties

Property code	Value	Unit	Source
hf	-42.56	kJ/mol	Joback Method
hvap	43.63	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.861		Crippen Method
mcvol	125.460	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
rinpol	1154.00		NIST Webbook
rinpol	1154.00		NIST Webbook
tb	531.10	K	Joback Method
tc	756.68	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R589678&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