

1,2-Propanedione, 1-phenyl-, 2-oxime

Other names:	2-(Hydroxyimino)propiophenone 1-Phenyl-1,2-propanedione 2-oxime «alpha»-Isonitrosopropiophenone «alpha»-Oximinopropiophenone Propiophenone, isonitroso- Isonitrosopropiophenone
Inchi:	InChI=1S/C9H9NO2/c1-7(10-12)9(11)8-5-3-2-4-6-8/h2-6,12H,1H3
InchiKey:	YPINLRNGSGGJJT-UHFFFAOYSA-N
Formula:	C9H9NO2
SMILES:	CC(=NO)C(=O)c1ccccc1
Mol. weight [g/mol]:	163.17
CAS:	119-51-7

Physical Properties

Property code	Value	Unit	Source
hf	-184.94	kJ/mol	Joback Method
hvap	64.72	kJ/mol	Joback Method
log10ws	-1.37		Crippen Method
logp	1.719		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	654.61	K	Joback Method
tc	876.07	K	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C119517&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

Latest version available from:

<https://www.cheméo.com/cid/33-320-9/1-2-Propanedione-1-phenyl-2-oxime.pdf>

Generated by Cheméo on 2024-04-29 22:47:56.558201521 +0000 UTC m=+16720125.478778833.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.