

1-Phenyl-1,2-propane-dione-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]:	163.18

Physical Properties

Property code	Value	Unit	Source
af	0.6407		Cheméo Relay (1.0)
gf	89.46	kJ/mol	Cheméo Relay (1.0, beta)
hf	-82.56	kJ/mol	Cheméo Relay (1.0)
hvap	76.47	kJ/mol	Cheméo Relay (1.0)
ie	9.13	eV	Cheméo Relay (1.0)
log10ws	-1.24		Cheméo Relay (1.0)
logp	1.719		Crippen Method
mcvol	127.030	ml/mol	McGowan Method
pc	3476.55	kPa	Joback Method
tb	553.98	K	Cheméo Relay (1.0)
tc	787.76	K	Cheméo Relay (1.0)
tf	370.64	K	Cheméo Relay (1.0)
vc	0.455	m3/kmol	Cheméo Relay (1.0)

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C119517&Units=SI>
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

af:	Acentric Factor
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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