

# Benzofuran-2,3-dione, 2-[O-(2-acetoxyethyl)oxime], 3-(O-methyloxime), isomer 1

InChI: [1S/C13H14N2O5/c1-9\(16\)18-7-8-19-15-13-12\(14-17-2\)10-5-3-4-6-11\(10\)20-13/h3](#)  
InChIKey: [MZOAUULLVZMEURP-UHFFFAOYSA-N](#)

Formula: C13H14N2O5

SMILES: CON=C1C(=NOCCOC(C)=O)Oc2ccccc21

Mol. weight [g/mol]: 278.26

## Physical Properties

Property code	Value	Unit	Source
hf	-552.63	kJ/mol	Joback Method
hvap	74.46	kJ/mol	Joback Method
log10ws	-1.91		Crippen Method
logp	1.323		Crippen Method
mcvol	195.820	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	2097.00		NIST Webbook
rinpol	2097.00		NIST Webbook
tb	846.31	K	Joback Method
tc	1077.59	K	Joback Method

## Sources

Joback Method: [https://en.wikipedia.org/wiki/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=R558822&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method: [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

hf: Enthalpy of formation at standard conditions

hvap: Enthalpy of vaporization at standard conditions

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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