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

InChI: 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: MZOAULLVZMEURP-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	2035.00		NIST Webbook
rinpol	2036.00		NIST Webbook
rinpol	2035.00		NIST Webbook
tb	846.31	K	Joback Method
tc	1077.59	K	Joback Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R558837&Units=SI

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