

5,6-Dihydro-1,4,2-dioxazin-3-yl)-(2-hydroxyphenyl)oxime, isomer 1

InChI: InChI=1S/C10H12N2O4/c13-8-4-2-1-3-7(8)9(11-14)10-12-16-6-5-15-10/h1-4,10,12-14H,1-2H2
InChIKey: SJZJUCGUKJOVTJ-UHFFFAOYSA-N

Formula: C10H12N2O4
SMILES: ON=C(c1ccccc1O)C1NOCCO1
Mol. weight [g/mol]: 224.21

Physical Properties

Property code	Value	Unit	Source
hf	-442.18	kJ/mol	Joback Method
hvap	89.42	kJ/mol	Joback Method
log10ws	-0.44		Crippen Method
logp	0.448		Crippen Method
mcvol	156.280	ml/mol	McGowan Method
pc	4480.21	kPa	Joback Method
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
tb	826.24	K	Joback Method
tc	1075.88	K	Joback Method

Sources

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>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R558862&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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