p-Benzoquinone 4-oxime

Inchi: InChI=1S/C6H5NO2/c8-6-3-1-5(7-9)2-4-6/h1-4,9H
InchiKey: KMGMCLWJFCGWFI-UHFFFAOYSA-N
Formula: C6H5NO2
SMILES: O=C1C=CC(=NO)C=C1
Mol. weight [g/mol]: 123.11
CAS: 637-62-7

Physical Properties

Property code	Value	Unit	Source
hf	-225.85	kJ/mol	Joback Method
hvap	55.34	kJ/mol	Joback Method
log10ws	-0.03		Crippen Method
logp	0.512		Crippen Method
mcvol	89.060	ml/mol	McGowan Method
pc	4534.68	kPa	Joback Method
tb	598.38	K	Joback Method
tc	828.42	K	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C637627&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature