

2,5-Cyclohexadiene-1,4-dione, dioxime

Other names:	p-Benzoquinone, dioxime p-Quinone dioxime p-Quinone oxime Benzoquinone dioxime Quinone dioxime 1,4-Benzoquinone dioxime Actor Q Dioxime p-benzoquinone Dioxime 1,4-cyclohexadienedione Dioxime 2,5-cyclohexadiene-1,4-dione NCI-C03850 1,4-Benzochinondioxim Dibenzo PQD G-M-F PQD QDO para-Quinone oxime 2,5-Cyclohexadiene-1,4-dione, 1,4-dioxime NSC 14433 NSC 4774 Vulnoc GM
Inchi:	InChI=1S/C6H6N2O2/c9-7-5-1-2-6(8-10)4-3-5/h1-4,9-10H
InchiKey:	LNHURPJLTHSVMU-UHFFFAOYSA-N
Formula:	C6H6N2O2
SMILES:	<chem>ON=C1C=CC(=NO)C=C1</chem>
Mol. weight [g/mol]:	138.12
CAS:	105-11-3

Physical Properties

Property code	Value	Unit	Source
hf	-199.35	kJ/mol	Joback Method
hvap	71.92	kJ/mol	Joback Method
log10ws	0.43		Crippen Method
logp	0.773		Crippen Method
mcvol	99.040	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method

tb	701.90	K	Joback Method
tc	914.45	K	Joback Method

Sources

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=C105113&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

hf:	Enthalpy of formation at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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