2,5-Cyclohexadien-1-one, 2,6-dichloro-4-(chloroimino)-

Other names: p-Benzoquinone imine, N,2,6-trichloro-
Gibbs reagent
N,2,6-Trichloro-p-benzoquinone imine
N,2,6-Trichlorobenzoquinone imine
2,6-Dichloro-4-N-chloroquinonimine
2,6-Dichlorobenzoquinone chloroimide
2,6-Dichloroquinone chloroimide
2,6-Dichloroquinone-4-chloroimide
2,6-Dichloroquinone-4-chloroimine
2,6-Dichloroquinone-4-chlorimide
2,6-Dichloro-p-benzoquinone-4-chlorimine
2,6-Dichloro-1,4-quinone-4-chlorimide
N-2,6-Trichloro-p-benzoquinonimine
2,5-Cyclohexadien-1-one, 4-chloroimino-2,6-dichloro-
2,6-Dichloroquinonechloroimine
4-Chloroimino-2,6-dichloro-2,5-cyclohexadiene-1-one
N,2,6-Trichloro-p-quinoneimine
2,6-Dichloro-4-(chloroimino)cyclohexa-2,5-dienone
NSC 6293
Gibbs' reagent

Inchi: InChI=1S/C6H2Cl3NO/c7-4-1-3(10-9)2-5(8)6(4)11/h1-2H

InchiKey: YHUMTHWQGWPJOQ-UHFFFAOYSA-N

Formula: C6H2Cl3NO

SMILES: O=C1C(Cl)=CC(=NCl)C=C1Cl

Mol. weight [g/mol]: 210.44

CAS: 101-38-2

Physical Properties

Property code	Value	Unit	Source
hf	-143.78	kJ/mol	Joback Method
hvap	53.14	kJ/mol	Joback Method
log10ws	-2.82		Crippen Method
logp	2.409		Crippen Method
mcvol	119.910	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
tb	628.45	K	Joback Method
tc	894.34	K	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101382&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