1,2-Naphthalenedione, 1-[(2-chlorophenyl)hydrozone]

Inchi: InChI=1S/C16H11ClN2O/c17-13-7-3-4-8-14(13)18-19-16-12-6-2-1-5-11(12)9-10-15(16)2

InchiKey: PRQXXWQHJWHDHV-MNDPQUGUSA-N

Formula: C16H11ClN2O

SMILES: O=C1C=Cc2ccccc2C1=NNc1ccccc1Cl

Mol. weight [g/mol]: 282.72

CAS: 74027-90-0

Physical Properties

Property code	Value	Unit	Source
hf	162.37	kJ/mol	Joback Method
hvap	76.98	kJ/mol	Joback Method
log10ws	-4.45		Crippen Method
logp	3.752		Crippen Method
mcvol	203.090	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
tb	878.22	K	Joback Method
tc	1153.22	K	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74027900&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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