(1E,2e)-1,3-bis(4-chlorophenyl)-2-buten-1-one oxime

Inchi: InChI=1S/C16H13Cl2NO/c1-11(12-2-6-14(17)7-3-12)10-16(19-20)13-4-8-15(18)9-5-13/h
InchiKey: SNCCPUZATGSEDC-WEGNKRRCSA-N
Formula: C16H13Cl2NO
SMILES: CC(=CC(=NO)c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]: 306.19
CAS: 30542-21-3

Physical Properties

Property code	Value	Unit	Source
hf	72.70	kJ/mol	Joback Method
hvap	85.97	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	5.275		Crippen Method
mcvol	220.510	ml/mol	McGowan Method
pc	2169.38	kPa	Joback Method
tb	876.44	K	Joback Method
tc	1121.92	K	Joback Method

Sources

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=C30542213&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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