

(1E)-1-(4-chlorophenyl)ethanone oxime

Inchi: InChI=1S/C8H8ClNO/c1-6(10-11)7-2-4-8(9)5-3-7/h2-5,11H,1H3/b10-6+
InchiKey: KAXTWDXRCMICEQ-UXBLZVDNSA-N
Formula: C8H8ClNO
SMILES: CC(=NO)c1ccc(Cl)cc1
Mol. weight [g/mol]: 169.61

Physical Properties

Property code	Value	Unit	Source
hf	-78.93	kJ/mol	Joback Method
hvap	60.80	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	2.538		Crippen Method
mcvol	123.610	ml/mol	McGowan Method
pc	3399.94	kPa	Joback Method
tb	620.27	K	Joback Method
tc	843.37	K	Joback Method

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=B6001469&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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