

E-3-(4-Chlorophenyl)-3-methoxyiminopropanenitrile

Inchi:	InChI=1S/C10H9ClN2O/c1-14-13-10(6-7-12)8-2-4-9(11)5-3-8/h2-5H,6H2,1H3
InchiKey:	BQWFIYSOMXQWBL-UHFFFAOYSA-N
Formula:	C10H9ClN2O
SMILES:	CON=C(CC#N)c1ccc(Cl)cc1
Mol. weight [g/mol]:	208.64

Physical Properties

Property code	Value	Unit	Source
hf	64.68	kJ/mol	Joback Method
hvap	61.46	kJ/mol	Joback Method
log10ws	-3.01		Crippen Method
logp	2.604		Crippen Method
mcpvol	153.170	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	1746.00		NIST Webbook
tb	698.35	K	Joback Method
tc	941.51	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=U373234&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

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