Oxirane-2,2-dicarbonitrile, 3-(2-chlorophenyl)-

Other names: Oxirane, 2,2-dicyano-3-(2-chlorophenyl)
Inchi: InChI=1S/C10H5ClN2O/c11-8-4-2-1-3-7(8)9-10(5-12,6-13)14-9/h1-4,9H
InchiKey: MVPVSDDVDXPOOP-UHFFFAOYSA-N
Formula: C10H5ClN2O
SMILES: N#CC1(C#N)OC1c1ccccc1Cl
Mol. weight [g/mol]: 204.61
CAS: 3513-08-4

Physical Properties

Property code	Value	Unit	Source
gf	351.96	kJ/mol	Joback Method
hf	225.05	kJ/mol	Joback Method
hfus	23.40	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-3.08		Crippen Method
logp	2.197		Crippen Method
mcvol	138.010	ml/mol	McGowan Method
pc	3032.27	kPa	Joback Method
rinpol	1366.00		NIST Webbook
rinpol	1366.00		NIST Webbook
tb	730.71	K	Joback Method
tc	993.53	K	Joback Method
tf	465.47	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.76	J/mol×K	730.71	Joback Method
cpg	340.55	J/mol×K	774.51	Joback Method
cpg	349.16	J/mol×K	818.32	Joback Method
cpg	357.83	J/mol×K	862.12	Joback Method
cpg	366.80	J/mol×K	905.92	Joback Method
cpg	376.30	J/mol×K	949.73	Joback Method

cpg	386.56	J/mol×K	993.53	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=C3513084&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion 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
tf:	Normal melting (fusion) point
vc:	Critical Volume