Propynenitrile, 3-(2-chlorophenyl)

Inchi: InChI=1S/C9H4ClN/c10-9-6-2-1-4-8(9)5-3-7-11/h1-2,4,6H
InchiKey: LVYSCYKCGCKDLQ-UHFFFAOYSA-N
Formula: C9H4ClN
SMILES: N#CC#Cc1ccccc1Cl
Mol. weight [g/mol]: 161.59

Physical Properties

Property code	Value	Unit	Source
gf	451.73	kJ/mol	Joback Method
hf	417.41	kJ/mol	Joback Method
hfus	21.54	kJ/mol	Joback Method
hvap	55.58	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	2.215		Crippen Method
mcvol	118.930	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	1338.00		NIST Webbook
tb	585.49	K	Joback Method
tc	849.33	K	Joback Method
tf	431.14	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	225.96	J/mol×K	585.49	Joback Method
cpg	234.81	J/mol×K	629.46	Joback Method
cpg	242.96	J/mol×K	673.44	Joback Method
cpg	250.46	J/mol×K	717.41	Joback Method
cpg	257.35	J/mol×K	761.38	Joback Method
cpg	263.66	J/mol×K	805.35	Joback Method
cpg	269.43	J/mol×K	849.33	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=R201417&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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