Prop-2-enenitrile, 3-(2-chlorophenyl)-

Other names: Cinnamonitrile, 2-chloro, trans
Inchi: InChI=1S/C9H6ClN/c10-9-6-2-1-4-8(9)5-3-7-11/h1-6H
InchiKey: PWWUUGALKZGDSD-UHFFFAOYSA-N
Formula: C9H6ClN
SMILES: N#CC=Cc1ccccc1Cl
Mol. weight [g/mol]: 163.60
CAS: 74738-21-9

Physical Properties

Property code	Value	Unit	Source
gf	329.15	kJ/mol	Joback Method
hf	262.33	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	53.39	kJ/mol	Joback Method
log10ws	-3.27		Crippen Method
logp	2.877		Crippen Method
mcvol	123.230	ml/mol	McGowan Method
pc	3170.40	kPa	Joback Method
rinpol	1424.00		NIST Webbook
tb	580.65	K	Joback Method
tc	824.26	K	Joback Method
tf	319.96	K	Joback Method
vc	0.486	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	245.87	J/mol×K	580.65	Joback Method
cpg	255.46	J/mol×K	621.25	Joback Method
cpg	264.29	J/mol×K	661.85	Joback Method
cpg	272.42	J/mol×K	702.46	Joback Method
cpg	279.91	J/mol×K	743.06	Joback Method
cpg	286.82	J/mol×K	783.66	Joback Method
cpg	293.20	J/mol×K	824.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74738219&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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