2-Chlorohydrocinnamonitrile

Other names:	Benzenepropanenitrile, 2-chloro- Hydrocinnamonitrile, o-chloro- 1-Cyano-2-(O-chlorophenyl)ethane 3-(2-Chlorophenyl)propanenitrile Propanenitrile, 3-(2-chlorophenyl)
Inchi:	InChI=1S/C9H8ClN/c10-9-6-2-1-4-8(9)5-3-7-11/h1-2,4,6H,3,5H2
InchiKey:	MMTXIUJWFHJGBA-UHFFFAOYSA-N
Formula:	C9H8ClN
SMILES:	N#CCCc1ccccc1Cl
Mol. weight [g/mol]:	165.62
CAS:	7315-17-5

Physical Properties

Property code	Value	Unit	Source
gf	248.93	kJ/mol	Joback Method
hf	145.11	kJ/mol	Joback Method
hfus	18.42	kJ/mol	Joback Method
hvap	53.43	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.796		Crippen Method
mcvol	127.530	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
rinpol	1368.00		NIST Webbook
tb	576.49	K	Joback Method
tc	809.28	K	Joback Method
tf	325.04	K	Joback Method
vc	0.506	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	266.26	J/mol×K	576.49	Joback Method
cpg	276.66	J/mol×K	615.29	Joback Method
cpg	286.34	J/mol×K	654.09	Joback Method

cpg	295.35	J/mol×K	692.89	Joback Method
cpg	303.72	J/mol×K	731.68	Joback Method
cpg	311.47	J/mol×K	770.48	Joback Method
cpg	318.66	J/mol×K	809.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7315175&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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