4-Cyanobenzoic acid, 3-chloroprop-2-enyl ester

Inchi: InChI=1S/C11H8ClNO2/c12-6-1-7-15-11(14)10-4-2-9(8-13)3-5-10/h1-6H,7H2/b6-1+

InchiKey: XVSJUDNOFHITQB-LZCJLJQNSA-N

Formula: C11H8ClNO2

SMILES: N#Cc1ccc(C(=O)OCC=CCl)cc1

Mol. weight [g/mol]: 221.64

Physical Properties

Property code	Value	Unit	Source
gf	112.07	kJ/mol	Joback Method
hf	-23.75	kJ/mol	Joback Method
hfus	26.59	kJ/mol	Joback Method
hvap	67.00	kJ/mol	Joback Method
log10ws	-3.41		Crippen Method
logp	2.468		Crippen Method
mcvol	158.850	ml/mol	McGowan Method
pc	2707.03	kPa	Joback Method
rinpol	1723.00		NIST Webbook
tb	702.70	K	Joback Method
tc	938.91	K	Joback Method
tf	414.66	K	Joback Method
vc	0.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	369.36	J/mol×K	702.70	Joback Method
cpg	379.24	J/mol×K	742.07	Joback Method
cpg	388.36	J/mol×K	781.44	Joback Method
cpg	396.75	J/mol×K	820.80	Joback Method
cpg	404.47	J/mol×K	860.17	Joback Method
cpg	411.54	J/mol×K	899.54	Joback Method
cpg	418.01	J/mol×K	938.91	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299231&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