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

Inchi: InChI=1S/C10H8Cl2O2/c11-6-1-7-14-10(13)8-2-4-9(12)5-3-8/h1-6H,7H2/b6-1+

InchiKey: KYSAXPAUQIXXNR-LZCJLJQNSA-N

Formula: C10H8Cl2O2

SMILES: O=C(OCC=CCl)c1ccc(Cl)cc1

Mol. weight [g/mol]: 231.07

Physical Properties

Property code	Value	Unit	Source
gf	-41.46	kJ/mol	Joback Method
hf	-183.73	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	58.68	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.249		Crippen Method
mcvol	155.620	ml/mol	McGowan Method
pc	2960.12	kPa	Joback Method
rinpol	1629.00		NIST Webbook
tb	615.17	K	Joback Method
tc	846.82	K	Joback Method
tf	368.32	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.06	J/mol×K	615.17	Joback Method
cpg	339.96	J/mol×K	653.78	Joback Method
cpg	350.08	J/mol×K	692.39	Joback Method
cpg	359.46	J/mol×K	731.00	Joback Method
cpg	368.12	J/mol×K	769.60	Joback Method
cpg	376.11	J/mol×K	808.21	Joback Method
cpg	383.47	J/mol×K	846.82	Joback Method
dvisc	0.0013966	Pa×s	368.32	Joback Method
dvisc	0.0008269	Pa×s	409.46	Joback Method

dvisc	0.0005387	Pa×s	450.60	Joback Method
dvisc	0.0003771	Pa×s	491.75	Joback Method
dvisc	0.0002789	Pa×s	532.89	Joback Method
dvisc	0.0002154	Pa×s	574.03	Joback Method
dvisc	0.0001722	Pa×s	615.17	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U299372&Units=SI

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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