2-Chlorobenzoic acid, allyl ester

Other names: Allyl 2-chlorobenzoate
Benzoic acid, 2-chloro, 2-propenyl ester
Inchi: InChI=1S/C10H9ClO2/c1-2-7-13-10(12)8-5-3-4-6-9(8)11/h2-6H,1,7H2
InchiKey: QAPRPPQBBCRDKG-UHFFFAOYSA-N
Formula: C10H9ClO2
SMILES: C=CCOC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 196.63
CAS: 7506-76-5

Physical Properties

Property code	Value	Unit	Source
gf	-21.91	kJ/mol	Joback Method
hf	-159.78	kJ/mol	Joback Method
hfus	21.01	kJ/mol	Joback Method
hvap	53.66	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.683		Crippen Method
mcvol	143.380	ml/mol	McGowan Method
pc	3049.04	kPa	Joback Method
rinpol	1420.00		NIST Webbook
rinpol	1396.00		NIST Webbook
rinpol	1403.00		NIST Webbook
rinpol	1407.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1399.00		NIST Webbook
rinpol	1407.00		NIST Webbook
ripol	2104.00		NIST Webbook
ripol	2094.00		NIST Webbook
ripol	2106.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2086.00		NIST Webbook
ripol	2127.00		NIST Webbook
ripol	2125.00		NIST Webbook
ripol	2086.00		NIST Webbook
tb	570.26	K	Joback Method
tc	793.10	K	Joback Method

tf	341.72	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	306.15	J/mol×K	570.26	Joback Method
cpg	317.89	J/mol×K	607.40	Joback Method
cpg	328.89	J/mol×K	644.54	Joback Method
cpg	339.18	J/mol×K	681.68	Joback Method
cpg	348.76	J/mol×K	718.82	Joback Method
cpg	357.67	J/mol×K	755.96	Joback Method
cpg	365.93	J/mol×K	793.10	Joback Method
dvisc	0.0016051	Pa×s	341.72	Joback Method
dvisc	0.0009722	Pa×s	379.81	Joback Method
dvisc	0.0006452	Pa×s	417.90	Joback Method
dvisc	0.0004585	Pa×s	455.99	Joback Method
dvisc	0.0003435	Pa×s	494.08	Joback Method
dvisc	0.0002682	Pa×s	532.17	Joback Method
dvisc	0.0002164	Pa×s	570.26	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=C7506765&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume