3-Chlorobenzoic acid, 2-chloroethyl ester

Other names: Benzoic acid, 3-chloro, 2-chloroethyl ester
Inchi: InChI=1S/C9H8Cl2O2/c10-4-5-13-9(12)7-2-1-3-8(11)6-7/h1-3,6H,4-5H2
InchiKey: ZVNHEUFAHIDPTB-UHFFFAOYSA-N
Formula: C9H8Cl2O2
SMILES: O=C(OCCCl)c1cccc(Cl)c1
Mol. weight [g/mol]: 219.06

Physical Properties

Property code	Value	Unit	Source
gf	-130.10	kJ/mol	Joback Method
hf	-280.31	kJ/mol	Joback Method
hfus	23.90	kJ/mol	Joback Method
hvap	56.49	kJ/mol	Joback Method
log10ws	-2.97		Crippen Method
logp	2.736		Crippen Method
mcvol	145.830	ml/mol	McGowan Method
pc	3107.10	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1551.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1537.00		NIST Webbook
tb	588.13	K	Joback Method
tc	814.30	K	Joback Method
tf	362.13	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	304.13	J/mol×K	588.13	Joback Method

cpg	350.97	J/mol×K	776.61	Joback Method
cpg	342.94	J/mol×K	738.91	Joback Method
cpg	334.25	J/mol×K	701.22	Joback Method
cpg	324.90	J/mol×K	663.52	Joback Method
cpg	314.86	J/mol×K	625.83	Joback Method
cpg	358.38	J/mol×K	814.30	Joback Method
dvisc	0.0002223	Pa×s	588.13	Joback Method
dvisc	0.0002757	Pa×s	550.46	Joback Method
dvisc	0.0003530	Pa×s	512.80	Joback Method
dvisc	0.0004699	Pa×s	475.13	Joback Method
dvisc	0.0006572	Pa×s	437.46	Joback Method
dvisc	0.0009791	Pa×s	399.80	Joback Method
dvisc	0.0015848	Pa×s	362.13	Joback Method

Sources

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=U357393&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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