2,2-Dichloroethyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, 2,2-dichloroethyl ester
Inchi: InChI=1S/C9H7Cl3O2/c10-7-3-1-2-6(4-7)9(13)14-5-8(11)12/h1-4,8H,5H2
InchiKey: HEQIZSUDEJTKNV-UHFFFAOYSA-N
Formula: C9H7Cl3O2
SMILES: O=C(OCC(Cl)Cl)c1cccc(Cl)c1
Mol. weight [g/mol]: 253.51

Physical Properties

Property code	Value	Unit	Source
gf	-144.47	kJ/mol	Joback Method
hf	-301.33	kJ/mol	Joback Method
hfus	24.57	kJ/mol	Joback Method
hvap	60.49	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.300		Crippen Method
mcvol	158.070	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	1643.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1618.00		NIST Webbook
rinpol	1683.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1624.00		NIST Webbook
rinpol	1632.00		NIST Webbook
rinpol	1618.00		NIST Webbook
tb	625.12	K	Joback Method
tc	859.74	K	Joback Method
tf	377.05	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.67	J/mol×K	625.12	Joback Method

cpg	336.80	J/mol×K	664.22	Joback Method
cpg	346.18	J/mol×K	703.33	Joback Method
cpg	354.82	J/mol×K	742.43	Joback Method
cpg	362.75	J/mol×K	781.53	Joback Method
cpg	369.99	J/mol×K	820.63	Joback Method
cpg	376.57	J/mol×K	859.74	Joback Method
dvisc	0.0017005	Pa×s	377.05	Joback Method
dvisc	0.0009910	Pa×s	418.39	Joback Method
dvisc	0.0006365	Pa×s	459.74	Joback Method
dvisc	0.0004397	Pa×s	501.09	Joback Method
dvisc	0.0003214	Pa×s	542.43	Joback Method
dvisc	0.0002456	Pa×s	583.77	Joback Method
dvisc	0.0001945	Pa×s	625.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373558&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
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