2-Chloroethyl benzoate

Other names: Benzoic acid 2-chloroethyl ester
Ethanol, 2-chloro-, benzoate
Inchi: InChI=1S/C9H9ClO2/c10-6-7-12-9(11)8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey: ANPPGQUFDXLAGY-UHFFFAOYSA-N
Formula: C9H9ClO2
SMILES: O=C(OCCCl)c1ccccc1
Mol. weight [g/mol]: 184.62
CAS: 939-55-9

Physical Properties

Property code	Value	Unit	Source
gf	-108.54	kJ/mol	Joback Method
hf	-253.10	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	51.44	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.082		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	1366.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1394.00		NIST Webbook
rinpol	1375.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1381.00		NIST Webbook
rinpol	1380.00		NIST Webbook
rinpol	1373.00		NIST Webbook
rinpol	1368.00		NIST Webbook
rinpol	1396.00		NIST Webbook
ripol	2137.00		NIST Webbook
ripol	2137.00		NIST Webbook
ripol	2101.00		NIST Webbook
ripol	2159.00		NIST Webbook
ripol	2137.00		NIST Webbook
tb	545.72	K	Joback Method
tc	766.71	K	Joback Method
tf	319.69	K	Joback Method

vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.46	J/mol×K	545.72	Joback Method
cpg	333.53	J/mol×K	729.88	Joback Method
cpg	324.51	J/mol×K	693.05	Joback Method
cpg	314.81	J/mol×K	656.22	Joback Method
cpg	304.41	J/mol×K	619.38	Joback Method
cpg	293.30	J/mol×K	582.55	Joback Method
cpg	341.89	J/mol×K	766.71	Joback Method
dvisc	0.0002345	Pa×s	545.72	Joback Method
dvisc	0.0002967	Pa×s	508.05	Joback Method
dvisc	0.0003898	Pa×s	470.38	Joback Method
dvisc	0.0005370	Pa×s	432.71	Joback Method
dvisc	0.0007864	Pa×s	395.03	Joback Method
dvisc	0.0012481	Pa×s	357.36	Joback Method
dvisc	0.0022086	Pa×s	319.69	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=C939559&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume