

2-Chlorobenzoic acid, 2-chloroethyl ester

Other names:	Benzoic acid, 2-chloro, 2-chloroethyl ester
Inchi:	InChI=1S/C9H8Cl2O2/c10-5-6-13-9(12)7-3-1-2-4-8(7)11/h1-4H,5-6H2
InchiKey:	OPAWQQDDCKSJAC-UHFFFAOYSA-N
Formula:	C9H8Cl2O2
SMILES:	O=C(OCCCl)c1ccccc1Cl
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	1549.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1552.00		NIST Webbook
rinpol	1541.00		NIST Webbook
rinpol	1538.00		NIST Webbook
rinpol	1540.00		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/molxK	588.13	Joback Method
cpg	350.97	J/molxK	776.61	Joback Method
cpg	342.94	J/molxK	738.91	Joback Method

cpg	334.25	J/molxK	701.22	Joback Method
cpg	324.90	J/molxK	663.52	Joback Method
cpg	314.86	J/molxK	625.83	Joback Method
cpg	358.38	J/molxK	814.30	Joback Method
dvisc	0.0002223	Paxs	588.13	Joback Method
dvisc	0.0002757	Paxs	550.46	Joback Method
dvisc	0.0003530	Paxs	512.80	Joback Method
dvisc	0.0004699	Paxs	475.13	Joback Method
dvisc	0.0006572	Paxs	437.46	Joback Method
dvisc	0.0009791	Paxs	399.80	Joback Method
dvisc	0.0015848	Paxs	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=U331323&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

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