2,2-Dichloroethyl benzoate

Other names:	Benzoic acid, 2,2-dichloroethyl ester
	Ethanol, 2,2-dichloro, benzoate
Inchi:	InChI=1S/C9H8Cl2O2/c10-8(11)6-13-9(12)7-4-2-1-3-5-7/h1-5,8H,6H2
InchiKey:	PQOOXAVSUMDZHX-UHFFFAOYSA-N
Formula:	C9H8Cl2O2
SMILES:	O=C(OCC(Cl)Cl)c1ccccc1
Mol. weight [g/mol]:	219.06

Physical Properties

Property code	Value	Unit	Source
gf	-122.91	kJ/mol	Joback Method
hf	-274.12	kJ/mol	Joback Method
hfus	20.77	kJ/mol	Joback Method
hvap	55.44	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.647		Crippen Method
mcvol	145.830	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	1462.00		NIST Webbook
rinpol	1485.00		NIST Webbook
rinpol	1470.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1459.00		NIST Webbook
rinpol	1453.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1472.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2192.00		NIST Webbook
ripol	2231.00		NIST Webbook
ripol	2226.00		NIST Webbook
ripol	2267.00		NIST Webbook
tb	582.71	K	Joback Method
tc	812.83	K	Joback Method
tf	334.61	K	Joback Method
vc	0.547	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	305.63	J/mol×K	582.71	Joback Method
cpg	316.93	J/mol×K	621.06	Joback Method
cpg	327.44	J/mol×K	659.42	Joback Method
cpg	337.17	J/mol×K	697.77	Joback Method
cpg	346.15	J/mol×K	736.13	Joback Method
cpg	354.41	J/mol×K	774.48	Joback Method
cpg	361.97	J/mol×K	812.83	Joback Method
dvisc	0.0025069	Pa×s	334.61	Joback Method
dvisc	0.0013249	Pa×s	375.96	Joback Method
dvisc	0.0007946	Pa×s	417.31	Joback Method
dvisc	0.0005225	Pa×s	458.66	Joback Method
dvisc	0.0003683	Pa×s	500.01	Joback Method
dvisc	0.0002738	Pa×s	541.36	Joback Method
dvisc	0.0002123	Pa×s	582.71	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=R31220&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