2,2,2-Trichloroethyl 3-chlorobenzoate

Other names: Benzoic acid, 3-chloro, 2,2,2-trichloroethyl ester
Inchi: InChI=1S/C9H6Cl4O2/c10-7-3-1-2-6(4-7)8(14)15-5-9(11,12)13/h1-4H,5H2
InchiKey: UDOKFBPXDCJNEF-UHFFFAOYSA-N
Formula: C9H6Cl4O2
SMILES: O=C(OCC(Cl)(Cl)Cl)c1cccc(Cl)c1
Mol. weight [g/mol]: 287.95

Physical Properties

Property code	Value	Unit	Source
gf	-151.12	kJ/mol	Joback Method
hf	-320.54	kJ/mol	Joback Method
hfus	24.88	kJ/mol	Joback Method
hvap	63.97	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.867		Crippen Method
mcvol	170.310	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	1744.00		NIST Webbook
rinpol	1705.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1688.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1690.00		NIST Webbook
rinpol	1678.00		NIST Webbook
tb	659.76	K	Joback Method
tc	906.78	K	Joback Method
tf	424.39	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.48	J/mol×K	659.76	Joback Method
cpg	359.71	J/mol×K	700.93	Joback Method

cpg	368.06	J/mol×K	742.10	Joback Method
cpg	375.59	J/mol×K	783.27	Joback Method
cpg	382.37	J/mol×K	824.44	Joback Method
cpg	388.45	J/mol×K	865.61	Joback Method
cpg	393.89	J/mol×K	906.78	Joback Method
dvisc	0.0012664	Pa×s	424.39	Joback Method
dvisc	0.0007795	Pa×s	463.62	Joback Method
dvisc	0.0005175	Pa×s	502.85	Joback Method
dvisc	0.0003646	Pa×s	542.08	Joback Method
dvisc	0.0002693	Pa×s	581.30	Joback Method
dvisc	0.0002066	Pa×s	620.53	Joback Method
dvisc	0.0001637	Pa×s	659.76	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373683&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