

4-Chlorobenzoic acid, 2,2,2-trichloroethyl ester

Other names:	Benzoic acid, 4-chloro, 2,2,2-trichloroethyl ester
Inchi:	InChI=1S/C9H6Cl4O2/c10-7-3-1-6(2-4-7)8(14)15-5-9(11,12)13/h1-4H,5H2
InchiKey:	SIPWACSQOMJEQO-UHFFFAOYSA-N
Formula:	C9H6Cl4O2
SMILES:	O=C(OCC(Cl)(Cl)Cl)c1ccc(Cl)cc1
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	1683.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1702.00		NIST Webbook
rinpol	1692.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1711.00		NIST Webbook
rinpol	1696.00		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/molxK	659.76	Joback Method
cpg	388.45	J/molxK	865.61	Joback Method

cpg	382.37	J/mol×K	824.44	Joback Method
cpg	375.59	J/mol×K	783.27	Joback Method
cpg	368.06	J/mol×K	742.10	Joback Method
cpg	359.71	J/mol×K	700.93	Joback Method
cpg	393.89	J/mol×K	906.78	Joback Method
dvisc	0.0001637	Paxs	659.76	Joback Method
dvisc	0.0002066	Paxs	620.53	Joback Method
dvisc	0.0002693	Paxs	581.30	Joback Method
dvisc	0.0003646	Paxs	542.08	Joback Method
dvisc	0.0005175	Paxs	502.85	Joback Method
dvisc	0.0007795	Paxs	463.62	Joback Method
dvisc	0.0012664	Paxs	424.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U354627&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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