Carbonic acid, 2,2,2-trichloroethyl 4-chlorophenyl ester

Inchi: InChI=1S/C9H6Cl4O3/c10-6-1-3-7(4-2-6)16-8(14)15-5-9(11,12)13/h1-4H,5H2

InchiKey: RETZDMQCOKIVNW-UHFFFAOYSA-N

Formula: C9H6Cl4O3

SMILES: O=C(OCC(Cl)(Cl)Cl)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 303.95

Physical Properties

Property code	Value	Unit	Source
gf	-256.12	kJ/mol	Joback Method
hf	-452.76	kJ/mol	Joback Method
hfus	26.07	kJ/mol	Joback Method
hvap	66.38	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.226		Crippen Method
mcvol	176.180	ml/mol	McGowan Method
pc	2871.95	kPa	Joback Method
rinpol	1825.00		NIST Webbook
tb	682.18	K	Joback Method
tc	925.19	K	Joback Method
tf	446.62	K	Joback Method
vc	0.658	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.26	J/mol×K	682.18	Joback Method
cpg	381.34	J/mol×K	722.68	Joback Method
cpg	389.57	J/mol×K	763.18	Joback Method
cpg	397.00	J/mol×K	803.69	Joback Method
cpg	403.65	J/mol×K	844.19	Joback Method
cpg	409.57	J/mol×K	884.69	Joback Method
cpg	414.77	J/mol×K	925.19	Joback Method
dvisc	0.0008978	Pa×s	446.62	Joback Method
dvisc	0.0005653	Pa×s	485.88	Joback Method

dvisc	0.0003815	Pa×s	525.14	Joback Method
dvisc	0.0002719	Pa×s	564.40	Joback Method
dvisc	0.0002025	Pa×s	603.66	Joback Method
dvisc	0.0001564	Pa×s	642.92	Joback Method
dvisc	0.0001244	Pa×s	682.18	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=U357900&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