Carbonic acid, 2,2,2-trichloroethyl 3,4-dichlorophenyl ester

Inchi: InChI=1S/C9H5Cl5O3/c10-6-2-1-5(3-7(6)11)17-8(15)16-4-9(12,13)14/h1-3H,4H2

InchiKey: ZLYNSNLAIUXXFY-UHFFFAOYSA-N

Formula: C9H5Cl5O3

SMILES: O=C(OCC(Cl)(Cl)Cl)Oc1ccc(Cl)c(Cl)c1

Mol. weight [g/mol]: 338.40

Physical Properties

Property code	Value	Unit	Source
gf	-277.68	kJ/mol	Joback Method
hf	-479.97	kJ/mol	Joback Method
hfus	29.88	kJ/mol	Joback Method
hvap	71.42	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.879		Crippen Method
mcvol	188.420	ml/mol	McGowan Method
pc	2718.33	kPa	Joback Method
rinpol	2006.00		NIST Webbook
tb	724.59	K	Joback Method
tc	970.75	K	Joback Method
tf	489.06	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.19	J/mol×K	724.59	Joback Method
cpg	397.09	J/mol×K	765.62	Joback Method
cpg	404.19	J/mol×K	806.64	Joback Method
cpg	410.54	J/mol×K	847.67	Joback Method
cpg	416.14	J/mol×K	888.70	Joback Method
cpg	421.04	J/mol×K	929.72	Joback Method
cpg	425.27	J/mol×K	970.75	Joback Method
dvisc	0.0006365	Pa×s	489.06	Joback Method
dvisc	0.0004239	Pa×s	528.32	Joback Method

dvisc	0.0002986	Pa×s	567.57	Joback Method
dvisc	0.0002201	Pa×s	606.83	Joback Method
dvisc	0.0001684	Pa×s	646.08	Joback Method
dvisc	0.0001328	Pa×s	685.34	Joback Method
dvisc	0.0001075	Pa×s	724.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357904&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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