Carbonochloridic acid, 2,2,2-trichloroethyl ester

Other names: Formic acid, chloro-, 2,2,2-trichloroethyl ester
Trichloroethyl chloroformate
2,2,2-Trichloroethoxycarbonyl chloride
2,2,2-Trichloroethyl chloroformate
Chloroformic acid 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C3H2Cl4O2/c4-2(8)9-1-3(5,6)7/h1H2

InchiKey: LJCZNYWLQZZIOS-UHFFFAOYSA-N

Formula: C3H2Cl4O2

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

Mol. weight [g/mol]: 211.86

CAS: 17341-93-4

Physical Properties

Property code	Value	Unit	Source
gf	-304.42	kJ/mol	Joback Method
hf	-421.76	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	47.67	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	2.732		Crippen Method
mcvol	109.530	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	444.70	K	NIST Webbook
tc	714.30	K	Joback Method
tf	317.83	K	Joback Method
vc	0.412	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.92	J/mol×K	490.82	Joback Method
cpg	198.16	J/mol×K	677.05	Joback Method
cpg	194.68	J/mol×K	639.81	Joback Method
cpg	190.84	J/mol×K	602.56	Joback Method

cpg	186.61	J/mol×K	565.31	Joback Method
cpg	181.98	J/mol×K	528.07	Joback Method
cpg	201.29	J/mol×K	714.30	Joback Method
dvisc	0.0003762	Pa×s	490.82	Joback Method
dvisc	0.0004782	Pa×s	461.99	Joback Method
dvisc	0.0006276	Pa×s	433.16	Joback Method
dvisc	0.0008562	Pa×s	404.33	Joback Method
dvisc	0.0012252	Pa×s	375.49	Joback Method
dvisc	0.0018609	Pa×s	346.66	Joback Method
dvisc	0.0030492	Pa×s	317.83	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C17341934&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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume