4-Chlorophenylchloro formate

Other names: p-Chlorophenyl chloroformate
Inchi: InChI=1S/C7H4Cl2O2/c8-5-1-3-6(4-2-5)11-7(9)10/h1-4H
InchiKey: RYWGPCLTVXMMHO-UHFFFAOYSA-N
Formula: C7H4Cl2O2
SMILES: O=C(Cl)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 191.01

Physical Properties

Property code	Value	Unit	Source
hf	-312.08	kJ/mol	Cheméo Relay (1.0)
hfus	18.72	kJ/mol	Joback Method
hvap	56.47	kJ/mol	Cheméo Relay (1.0)
ie	8.99	eV	Cheméo Relay (1.0)
log10ws	-3.51		Cheméo Relay (1.0)
logp	3.078		Crippen Method
mcvol	117.650	ml/mol	McGowan Method
tb	495.50	K	Cheméo Relay (1.0)
tf	273.87	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.11	J/mol×K	542.37	Joback Method
cpg	225.62	J/mol×K	581.56	Joback Method
cpg	233.56	J/mol×K	620.75	Joback Method
cpg	240.95	J/mol×K	659.94	Joback Method
cpg	247.78	J/mol×K	699.13	Joback Method
cpg	254.07	J/mol×K	738.32	Joback Method
cpg	259.83	J/mol×K	777.51	Joback Method
dvisc	0.0016588	Pa×s	339.59	Joback Method
dvisc	0.0010650	Pa×s	373.39	Joback Method
dvisc	0.0007359	Pa×s	407.18	Joback Method
dvisc	0.0005382	Pa×s	440.98	Joback Method
dvisc	0.0004115	Pa×s	474.78	Joback Method

dvisc	0.0003261	Pa×s	508.57	Joback Method
dvisc	0.0002660	Pa×s	542.37	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	379.00 ± 1.00	K	2.10	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C7693450&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point