chloromethyl dichloroacetate

Inchi: InChI=1S/C3H3Cl3O2/c4-1-8-3(7)2(5)6/h2H,1H2
InchiKey: FVCUMUOCIBFJLZ-UHFFFAOYSA-N
Formula: C3H3Cl3O2
SMILES: O=C(OCCl)C(Cl)Cl
Mol. weight [g/mol]: 177.41

Physical Properties

Property code	Value	Unit	Source
gf	-297.77	kJ/mol	Joback Method
hf	-402.55	kJ/mol	Joback Method
hfus	15.38	kJ/mol	Joback Method
hvap	44.19	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	1.530		Crippen Method
mcvol	97.290	ml/mol	McGowan Method
pc	4093.38	kPa	Joback Method
rinpol	960.00		NIST Webbook
rinpol	976.00		NIST Webbook
rinpol	962.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	926.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1705.00		NIST Webbook
ripol	1687.00		NIST Webbook
ripol	1700.00		NIST Webbook
tb	456.18	K	Joback Method
tc	664.45	K	Joback Method
tf	270.49	K	Joback Method
vc	0.368	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	155.51	J/mol×K	456.18	Joback Method
cpg	160.55	J/mol×K	490.89	Joback Method
cpg	165.36	J/mol×K	525.60	Joback Method
cpg	169.94	J/mol×K	560.31	Joback Method
cpg	174.30	J/mol×K	595.02	Joback Method
cpg	178.42	J/mol×K	629.73	Joback Method
cpg	182.30	J/mol×K	664.45	Joback Method
dvisc	0.0036245	Pa×s	270.49	Joback Method
dvisc	0.0020410	Pa×s	301.44	Joback Method
dvisc	0.0012790	Pa×s	332.39	Joback Method
dvisc	0.0008680	Pa×s	363.34	Joback Method
dvisc	0.0006260	Pa×s	394.28	Joback Method
dvisc	0.0004734	Pa×s	425.23	Joback Method
dvisc	0.0003719	Pa×s	456.18	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R112639&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume