Chloroacetic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C8H6Cl2O2/c9-5-8(11)12-7-3-1-6(10)2-4-7/h1-4H,5H2
InchiKey: GEQGYTKAVRDKNR-UHFFFAOYSA-N
Formula: C8H6Cl2O2
SMILES: O=C(CCl)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 205.04

Physical Properties

Property code	Value	Unit	Source
gf	-138.52	kJ/mol	Joback Method
hf	-259.67	kJ/mol	Joback Method
hfus	21.31	kJ/mol	Joback Method
hvap	54.27	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.484		Crippen Method
mcvol	131.740	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1424.00		NIST Webbook
tb	565.25	K	Joback Method
tc	795.82	K	Joback Method
tf	350.86	K	Joback Method
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.71	J/mol×K	565.25	Joback Method
cpg	301.95	J/mol×K	757.40	Joback Method
cpg	294.73	J/mol×K	718.97	Joback Method
cpg	286.90	J/mol×K	680.54	Joback Method
cpg	278.47	J/mol×K	642.11	Joback Method
cpg	269.41	J/mol×K	603.68	Joback Method
cpg	308.59	J/mol×K	795.82	Joback Method
dvisc	0.0002441	Pa×s	565.25	Joback Method
dvisc	0.0003011	Pa×s	529.52	Joback Method

dvisc	0.0003828	Pa×s	493.79	Joback Method
dvisc	0.0005053	Pa×s	458.06	Joback Method
dvisc	0.0006989	Pa×s	422.32	Joback Method
dvisc	0.0010266	Pa×s	386.59	Joback Method
dvisc	0.0016308	Pa×s	350.86	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307712&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

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