Phenyl «beta»-chloropropionate

Other names:	«beta»-Chloropropionic acid phenyl ester
	3-Chloropropionic acid, phenyl ester
Inchi:	InChI=1S/C9H9ClO2/c10-7-6-9(11)12-8-4-2-1-3-5-8/h1-5H,6-7H2
InchiKey:	RAFRTSDUWORDLA-UHFFFAOYSA-N
Formula:	C9H9ClO2
SMILES:	O=C(CCCl)Oc1ccccc1
Mol. weight [g/mol]:	184.62
CAS:	24552-27-0

Physical Properties

Property code	Value	Unit	Source
gf	-108.54	kJ/mol	Joback Method
hf	-253.10	kJ/mol	Joback Method
hfus	20.09	kJ/mol	Joback Method
hvap	51.44	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.221		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	545.72	K	Joback Method
tc	766.71	K	Joback Method
tf	319.69	K	Joback Method
vc	0.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.46	J/mol×K	545.72	Joback Method
cpg	293.30	J/mol×K	582.55	Joback Method
cpg	304.41	J/mol×K	619.38	Joback Method
cpg	314.81	J/mol×K	656.22	Joback Method
cpg	324.51	J/mol×K	693.05	Joback Method
cpg	333.53	J/mol×K	729.88	Joback Method
cpg	341.89	J/mol×K	766.71	Joback Method

dvisc	0.0022086	Pa×s	319.69	Joback Method
dvisc	0.0012481	Pa×s	357.36	Joback Method
dvisc	0.0007864	Pa×s	395.03	Joback Method
dvisc	0.0005370	Pa×s	432.71	Joback Method
dvisc	0.0003898	Pa×s	470.38	Joback Method
dvisc	0.0002967	Pa×s	508.05	Joback Method
dvisc	0.0002345	Pa×s	545.72	Joback Method

Sources

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=C24552270&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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