2-Chloropropionic acid, phenyl ester

Inchi: InChI=1S/C9H9ClO2/c1-7(10)9(11)12-8-5-3-2-4-6-8/h2-7H,1H3
InchiKey: PTFWCFRZCGETRS-UHFFFAOYSA-N
Formula: C9H9ClO2
SMILES: CC(Cl)C(=O)Oc1ccccc1
Mol. weight [g/mol]: 184.62

Physical Properties

Property code	Value	Unit	Source
gf	-110.98	kJ/mol	Joback Method
hf	-258.38	kJ/mol	Joback Method
hfus	16.57	kJ/mol	Joback Method
hvap	51.06	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.219		Crippen Method
mcvol	133.590	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
rinpol	1287.00		NIST Webbook
tb	545.28	K	Joback Method
tc	771.28	K	Joback Method
tf	304.69	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.82	J/mol×K	545.28	Joback Method
cpg	335.15	J/mol×K	733.61	Joback Method
cpg	325.96	J/mol×K	695.95	Joback Method
cpg	316.05	J/mol×K	658.28	Joback Method
cpg	305.41	J/mol×K	620.61	Joback Method
cpg	294.01	J/mol×K	582.95	Joback Method
cpg	343.63	J/mol×K	771.28	Joback Method
dvisc	0.0002204	Pa×s	545.28	Joback Method
dvisc	0.0002851	Pa×s	505.18	Joback Method

dvisc	0.0003856	Pa×s	465.08	Joback Method
dvisc	0.0005521	Pa×s	424.99	Joback Method
dvisc	0.0008517	Pa×s	384.89	Joback Method
dvisc	0.0014534	Pa×s	344.79	Joback Method
dvisc	0.0028549	Pa×s	304.69	Joback Method

Sources

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=U357775&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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