2,2-Dimethylpropanoic acid, 4-chlorophenyl ester

Inchi: InChI=1S/C11H13ClO2/c1-11(2,3)10(13)14-9-6-4-8(12)5-7-9/h4-7H,1-3H3
InchiKey: OYQBAUOEQCWQJN-UHFFFAOYSA-N
Formula: C11H13ClO2
SMILES: CC(C)(C)C(=O)Oc1ccc(Cl)cc1
Mol. weight [g/mol]: 212.67

Physical Properties

Property code	Value	Unit	Source
gf	-98.49	kJ/mol	Joback Method
hf	-314.60	kJ/mol	Joback Method
hfus	17.47	kJ/mol	Joback Method
hvap	55.26	kJ/mol	Joback Method
log10ws	-3.48		Crippen Method
logp	3.291		Crippen Method
mcvol	161.770	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
rinpol	1379.00		NIST Webbook
tb	593.23	K	Joback Method
tc	820.88	K	Joback Method
tf	357.17	K	Joback Method
vc	0.606	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.31	J/mol×K	593.23	Joback Method
cpg	390.36	J/mol×K	631.17	Joback Method
cpg	403.42	J/mol×K	669.11	Joback Method
cpg	415.54	J/mol×K	707.05	Joback Method
cpg	426.78	J/mol×K	744.99	Joback Method
cpg	437.16	J/mol×K	782.93	Joback Method
cpg	446.75	J/mol×K	820.88	Joback Method
dvisc	0.0017948	Pa×s	357.17	Joback Method
dvisc	0.0009991	Pa×s	396.51	Joback Method

dvisc	0.0006182	Pa×s	435.86	Joback Method
dvisc	0.0004142	Pa×s	475.20	Joback Method
dvisc	0.0002950	Pa×s	514.54	Joback Method
dvisc	0.0002205	Pa×s	553.89	Joback Method
dvisc	0.0001713	Pa×s	593.23	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=U308040&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume