2,2-Dimethylpropanoic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C11H12Cl2O2/c1-11(2,3)10(14)15-7-4-5-8(12)9(13)6-7/h4-6H,1-3H3
InchiKey: XIRSVOKAKYHVOX-UHFFFAOYSA-N
Formula: C11H12Cl2O2
SMILES: CC(C)(C)C(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 247.12

Physical Properties

Property code	Value	Unit	Source
gf	-120.05	kJ/mol	Joback Method
hf	-341.81	kJ/mol	Joback Method
hfus	21.28	kJ/mol	Joback Method
hvap	60.31	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	3.945		Crippen Method
mcvol	174.010	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1552.00		NIST Webbook
rinpol	1552.00		NIST Webbook
tb	635.64	K	Joback Method
tc	867.66	K	Joback Method
tf	399.61	K	Joback Method
vc	0.654	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	400.40	J/mol×K	635.64	Joback Method
cpg	413.12	J/mol×K	674.31	Joback Method
cpg	424.92	J/mol×K	712.98	Joback Method
cpg	435.84	J/mol×K	751.65	Joback Method
cpg	445.91	J/mol×K	790.32	Joback Method
cpg	455.19	J/mol×K	828.99	Joback Method
cpg	463.72	J/mol×K	867.66	Joback Method
dvisc	0.0012318	Pa×s	399.61	Joback Method

dvisc	0.0007473	Pa×s	438.95	Joback Method
dvisc	0.0004922	Pa×s	478.29	Joback Method
dvisc	0.0003454	Pa×s	517.62	Joback Method
dvisc	0.0002548	Pa×s	556.96	Joback Method
dvisc	0.0001957	Pa×s	596.30	Joback Method
dvisc	0.0001553	Pa×s	635.64	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=U308044&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume