Acetoxyacetic acid, 3,4-dichlorophenyl ester

Inchi: InChI=1S/C10H8Cl2O4/c1-6(13)15-5-10(14)16-7-2-3-8(11)9(12)4-7/h2-4H,5H2,1H3
InchiKey: ISETXWLPWNBHGV-UHFFFAOYSA-N
Formula: C10H8Cl2O4
SMILES: CC(=O)OCC(=O)Oc1ccc(Cl)c(Cl)c1
Mol. weight [g/mol]: 263.07

Physical Properties

Property code	Value	Unit	Source
gf	-365.23	kJ/mol	Joback Method
hf	-557.22	kJ/mol	Joback Method
hfus	28.89	kJ/mol	Joback Method
hvap	68.54	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.462		Crippen Method
mcvol	167.360	ml/mol	McGowan Method
pc	2893.62	kPa	Joback Method
rinpol	1722.00		NIST Webbook
rinpol	1722.00		NIST Webbook
tb	692.28	K	Joback Method
tc	918.63	K	Joback Method
tf	458.08	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.52	J/mol×K	692.28	Joback Method
cpg	425.09	J/mol×K	880.90	Joback Method
cpg	418.06	J/mol×K	843.18	Joback Method
cpg	410.29	J/mol×K	805.45	Joback Method
cpg	401.77	J/mol×K	767.73	Joback Method
cpg	392.51	J/mol×K	730.00	Joback Method
cpg	431.35	J/mol×K	918.63	Joback Method
dvisc	0.0001585	Pa×s	692.28	Joback Method

dvisc	0.0001926	Pa×s	653.25	Joback Method
dvisc	0.0002401	Pa×s	614.21	Joback Method
dvisc	0.0003082	Pa×s	575.18	Joback Method
dvisc	0.0004104	Pa×s	536.15	Joback Method
dvisc	0.0005716	Pa×s	497.11	Joback Method
dvisc	0.0008424	Pa×s	458.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307544&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