Chloroacetic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C8H4Cl4O2/c9-3-8(13)14-7-2-5(11)4(10)1-6(7)12/h1-2H,3H2
InchiKey: HERRLRXZMJPBFQ-UHFFFAOYSA-N
Formula: C8H4Cl4O2
SMILES: O=C(CCl)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 273.93

Physical Properties

Property code	Value	Unit	Source
gf	-181.64	kJ/mol	Joback Method
hf	-314.09	kJ/mol	Joback Method
hfus	28.93	kJ/mol	Joback Method
hvap	64.36	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.791		Crippen Method
mcvol	156.220	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	1774.00		NIST Webbook
tb	650.07	K	Joback Method
tc	889.48	K	Joback Method
tf	435.74	K	Joback Method
vc	0.596	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	296.81	J/mol×K	650.07	Joback Method
cpg	329.57	J/mol×K	849.58	Joback Method
cpg	324.15	J/mol×K	809.68	Joback Method
cpg	318.17	J/mol×K	769.78	Joback Method
cpg	311.62	J/mol×K	729.87	Joback Method
cpg	304.50	J/mol×K	689.97	Joback Method
cpg	334.44	J/mol×K	889.48	Joback Method
dvisc	0.0002109	Pa×s	650.07	Joback Method
dvisc	0.0002521	Pa×s	614.35	Joback Method

dvisc	0.0003081	Pa×s	578.63	Joback Method
dvisc	0.0003867	Pa×s	542.90	Joback Method
dvisc	0.0005010	Pa×s	507.18	Joback Method
dvisc	0.0006752	Pa×s	471.46	Joback Method
dvisc	0.0009555	Pa×s	435.74	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=U354613&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