Dimethylmalonic acid, monochloride, 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C11H8Cl4O3/c1-11(2,9(15)16)10(17)18-7-4-5(12)3-6(13)8(7)14/h3-4H,1-2H3
InchiKey: GEICBZKFGWZMCW-UHFFFAOYSA-N
Formula: C11H8Cl4O3
SMILES: CC(C)(C(=O)Cl)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 329.99

Physical Properties

Property code	Value	Unit	Source
gf	-282.46	kJ/mol	Joback Method
hf	-497.34	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	76.49	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.344		Crippen Method
mcvol	200.060	ml/mol	McGowan Method
pc	2480.12	kPa	Joback Method
rinpol	1991.00		NIST Webbook
rinpol	1991.00		NIST Webbook
tb	769.35	K	Joback Method
tc	1012.85	K	Joback Method
tf	521.90	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	450.46	J/mol×K	769.35	Joback Method
cpg	459.30	J/mol×K	809.93	Joback Method
cpg	467.30	J/mol×K	850.52	Joback Method
cpg	474.51	J/mol×K	891.10	Joback Method
cpg	480.97	J/mol×K	931.68	Joback Method
cpg	486.72	J/mol×K	972.27	Joback Method
cpg	491.81	J/mol×K	1012.85	Joback Method
dvisc	0.0006544	Pa×s	521.90	Joback Method

dvisc	0.0004439	Pa×s	563.14	Joback Method
dvisc	0.0003175	Pa×s	604.38	Joback Method
dvisc	0.0002370	Pa×s	645.62	Joback Method
dvisc	0.0001832	Pa×s	686.87	Joback Method
dvisc	0.0001459	Pa×s	728.11	Joback Method
dvisc	0.0001190	Pa×s	769.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363913&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