Dimethylmalonic acid, 2,3-dichlorophenyl propyl ester

Inchi: InChI=1S/C14H16Cl2O4/c1-4-8-19-12(17)14(2,3)13(18)20-10-7-5-6-9(15)11(10)16/h5-7H

InchiKey: WYUWYJZKWBVDHB-UHFFFAOYSA-N

Formula: C14H16Cl2O4

SMILES: CCCOC(=O)C(C)(C)C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 319.18

Physical Properties

Property code	Value	Unit	Source
gf	-328.71	kJ/mol	Joback Method
hf	-648.53	kJ/mol	Joback Method
hfus	31.83	kJ/mol	Joback Method
hvap	76.14	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.878		Crippen Method
mcvol	223.720	ml/mol	McGowan Method
pc	2021.76	kPa	Joback Method
rinpol	2001.00		NIST Webbook
rinpol	2001.00		NIST Webbook
tb	780.57	K	Joback Method
tc	1003.61	K	Joback Method
tf	505.58	K	Joback Method
vc	0.847	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.06	J/mol×K	780.57	Joback Method
cpg	603.39	J/mol×K	817.74	Joback Method
cpg	614.74	J/mol×K	854.92	Joback Method
cpg	625.11	J/mol×K	892.09	Joback Method
cpg	634.55	J/mol×K	929.26	Joback Method
cpg	643.09	J/mol×K	966.44	Joback Method
cpg	650.75	J/mol×K	1003.61	Joback Method
dvisc	0.0005761	Pa×s	505.58	Joback Method

dvisc	0.0003589	Pa×s	551.41	Joback Method
dvisc	0.0002404	Pa×s	597.24	Joback Method
dvisc	0.0001705	Pa×s	643.07	Joback Method
dvisc	0.0001266	Pa×s	688.91	Joback Method
dvisc	0.0000975	Pa×s	734.74	Joback Method
dvisc	0.0000775	Pa×s	780.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363620&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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