Dimethylmalonic acid, propyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C14H15Cl3O4/c1-4-5-20-12(18)14(2,3)13(19)21-11-9(16)6-8(15)7-10(11)17/h6

InchiKey: VULSHHCHBHVVTO-UHFFFAOYSA-N

Formula: C14H15Cl3O4

SMILES: CCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 353.62

Physical Properties

Property code	Value	Unit	Source
gf	-350.27	kJ/mol	Joback Method
hf	-675.74	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	81.19	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.532		Crippen Method
mcvol	235.960	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
tb	822.98	K	Joback Method
tc	1049.66	K	Joback Method
tf	548.02	K	Joback Method
vc	0.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	611.60	J/mol×K	822.98	Joback Method
cpg	622.67	J/mol×K	860.76	Joback Method
cpg	632.78	J/mol×K	898.54	Joback Method
cpg	641.93	J/mol×K	936.32	Joback Method
cpg	650.15	J/mol×K	974.10	Joback Method
cpg	657.48	J/mol×K	1011.88	Joback Method
cpg	663.93	J/mol×K	1049.66	Joback Method
dvisc	0.0004186	Pa×s	548.02	Joback Method

dvisc	0.0002744	Pa×s	593.85	Joback Method
dvisc	0.0001911	Pa×s	639.67	Joback Method
dvisc	0.0001397	Pa×s	685.50	Joback Method
dvisc	0.0001062	Pa×s	731.33	Joback Method
dvisc	0.0000834	Pa×s	777.15	Joback Method
dvisc	0.0000672	Pa×s	822.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363645&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