Dimethylmalonic acid, 2,5-dichlorophenyl tridecyl ester

Inchi: InChI=1S/C24H36Cl2O4/c1-4-5-6-7-8-9-10-11-12-13-14-17-29-22(27)24(2,3)23(28)30-21
InchiKey: JTVDPVLQRPHJKJ-UHFFFAOYSA-N
Formula: C24H36Cl2O4
SMILES: CCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 459.45

Physical Properties

Property code	Value	Unit	Source
gf	-244.51	kJ/mol	Joback Method
hf	-854.93	kJ/mol	Joback Method
hfus	57.73	kJ/mol	Joback Method
hvap	98.40	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.779		Crippen Method
mcvol	364.620	ml/mol	McGowan Method
pc	986.40	kPa	Joback Method
rinpol	2904.00		NIST Webbook
tb	1009.37	K	Joback Method
tc	1235.86	K	Joback Method
tf	618.28	K	Joback Method
vc	1.407	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.80	J/mol×K	1009.37	Joback Method
cpg	1230.52	J/mol×K	1198.11	Joback Method
cpg	1220.75	J/mol×K	1160.37	Joback Method
cpg	1209.87	J/mol×K	1122.62	Joback Method
cpg	1197.79	J/mol×K	1084.87	Joback Method
cpg	1184.46	J/mol×K	1047.12	Joback Method
cpg	1239.24	J/mol×K	1235.86	Joback Method
dvisc	0.0000168	Pa×s	1009.37	Joback Method
dvisc	0.0000218	Pa×s	944.19	Joback Method

dvisc	0.0000294	Pa×s	879.01	Joback Method
dvisc	0.0000417	Pa×s	813.82	Joback Method
dvisc	0.0000628	Pa×s	748.64	Joback Method
dvisc	0.0001021	Pa×s	683.46	Joback Method
dvisc	0.0001841	Pa×s	618.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U363690&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