Dimethylmalonic acid, 2,5-dichlorophenyl hexadecyl ester

Inchi: InChI=1S/C27H42Cl2O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-32-25(30)27(2,3)26
InchiKey: VTRHGLRVIXYCGG-UHFFFAOYSA-N
Formula: C27H42Cl2O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1cc(Cl)ccc1Cl
Mol. weight [g/mol]: 501.53

Physical Properties

Property code	Value	Unit	Source
gf	-219.25	kJ/mol	Joback Method
hf	-916.85	kJ/mol	Joback Method
hfus	65.50	kJ/mol	Joback Method
hvap	105.08	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	8.950		Crippen Method
mcvol	406.890	ml/mol	McGowan Method
pc	829.55	kPa	Joback Method
rinpol	3226.00		NIST Webbook
rinpol	3226.00		NIST Webbook
tb	1078.01	K	Joback Method
tc	1323.54	K	Joback Method
tf	652.09	K	Joback Method
vc	1.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1355.04	J/mol×K	1078.01	Joback Method
cpg	1418.34	J/mol×K	1282.61	Joback Method
cpg	1408.37	J/mol×K	1241.69	Joback Method
cpg	1397.16	J/mol×K	1200.77	Joback Method
cpg	1384.60	J/mol×K	1159.85	Joback Method
cpg	1370.60	J/mol×K	1118.93	Joback Method
cpg	1427.16	J/mol×K	1323.54	Joback Method
dvisc	0.0000103	Pa×s	1078.01	Joback Method

dvisc	0.0000135	Pa×s	1007.02	Joback Method
dvisc	0.0000184	Pa×s	936.04	Joback Method
dvisc	0.0000263	Pa×s	865.05	Joback Method
dvisc	0.0000402	Pa×s	794.06	Joback Method
dvisc	0.0000668	Pa×s	723.08	Joback Method
dvisc	0.0001238	Pa×s	652.09	Joback Method

Sources

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=U363693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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