Diethylmalonic acid, 2,6-dichlorophenyl heptadecyl ester

Inchi: InChI=1S/C30H48Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-24-35-28(33)30(
InchiKey: HHVHCEWKCKXVMH-UHFFFAOYSA-N
Formula: C30H48Cl2O4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 543.61

Physical Properties

Property code	Value	Unit	Source
gf	-193.99	kJ/mol	Joback Method
hf	-978.77	kJ/mol	Joback Method
hfus	73.27	kJ/mol	Joback Method
hvap	111.76	kJ/mol	Joback Method
log10ws	-10.99		Crippen Method
logp	10.120		Crippen Method
mcvol	449.160	ml/mol	McGowan Method
pc	707.33	kPa	Joback Method
rinpol	3561.00		NIST Webbook
tb	1146.65	K	Joback Method
tc	1422.95	K	Joback Method
tf	685.90	K	Joback Method
vc	1.742	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1543.56	J/mol×K	1146.65	Joback Method
cpg	1560.40	J/mol×K	1192.70	Joback Method
cpg	1575.35	J/mol×K	1238.75	Joback Method
cpg	1588.60	J/mol×K	1284.80	Joback Method
cpg	1600.29	J/mol×K	1330.85	Joback Method
cpg	1610.61	J/mol×K	1376.90	Joback Method
cpg	1619.70	J/mol×K	1422.95	Joback Method
dvisc	0.0000818	Pa×s	685.90	Joback Method
dvisc	0.0000430	Pa×s	762.69	Joback Method

dvisc	0.0000254	Pa×s	839.48	Joback Method
dvisc	0.0000164	Pa×s	916.27	Joback Method
dvisc	0.0000113	Pa×s	993.07	Joback Method
dvisc	0.0000082	Pa×s	1069.86	Joback Method
dvisc	0.0000063	Pa×s	1146.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369944&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