Diethylmalonic acid, 3,5-dichlorophenyl hexadecyl ester

Inchi: InChI=1S/C29H46Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-34-27(32)29(5-2
InchiKey: UFNQRMWBKXDYRR-UHFFFAOYSA-N
Formula: C29H46Cl2O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 529.58

Physical Properties

Property code	Value	Unit	Source
gf	-202.41	kJ/mol	Joback Method
hf	-958.13	kJ/mol	Joback Method
hfus	70.68	kJ/mol	Joback Method
hvap	109.53	kJ/mol	Joback Method
log10ws	-10.57		Crippen Method
logp	9.730		Crippen Method
mcvol	435.070	ml/mol	McGowan Method
pc	744.88	kPa	Joback Method
rinpol	3343.00		NIST Webbook
tb	1123.77	K	Joback Method
tc	1388.35	K	Joback Method
tf	674.63	K	Joback Method
vc	1.687	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1480.41	J/mol×K	1123.77	Joback Method
cpg	1496.77	J/mol×K	1167.87	Joback Method
cpg	1511.37	J/mol×K	1211.96	Joback Method
cpg	1524.35	J/mol×K	1256.06	Joback Method
cpg	1535.86	J/mol×K	1300.16	Joback Method
cpg	1546.03	J/mol×K	1344.25	Joback Method
cpg	1555.00	J/mol×K	1388.35	Joback Method
dvisc	0.0000941	Pa×s	674.63	Joback Method
dvisc	0.0000498	Pa×s	749.49	Joback Method

dvisc	0.0000296	Pa×s	824.34	Joback Method
dvisc	0.0000192	Pa×s	899.20	Joback Method
dvisc	0.0000133	Pa×s	974.06	Joback Method
dvisc	0.0000097	Pa×s	1048.91	Joback Method
dvisc	0.0000074	Pa×s	1123.77	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U370447&Units=SI

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