Diethylmalonic acid, 4-chloro-3-methylphenyl heptadecyl ester

Inchi: InChI=1S/C31H51ClO4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-21-24-35-29(33)31(
InchiKey: JFCAIWWJBHOHKD-UHFFFAOYSA-N
Formula: C31H51ClO4
SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1
Mol. weight [g/mol]: 523.19

Physical Properties

Property code	Value	Unit	Source
gf	-173.64	kJ/mol	Joback Method
hf	-983.67	kJ/mol	Joback Method
hfus	71.67	kJ/mol	Joback Method
hvap	109.60	kJ/mol	Joback Method
log10ws	-10.78		Crippen Method
logp	9.775		Crippen Method
mcvol	451.010	ml/mol	McGowan Method
pc	685.65	kPa	Joback Method
rinpol	3500.00		NIST Webbook
tb	1132.10	K	Joback Method
tc	1406.24	K	Joback Method
tf	667.25	K	Joback Method
vc	1.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1584.53	J/mol×K	1132.10	Joback Method
cpg	1602.84	J/mol×K	1177.79	Joback Method
cpg	1619.14	J/mol×K	1223.48	Joback Method
cpg	1633.61	J/mol×K	1269.17	Joback Method
cpg	1646.40	J/mol×K	1314.86	Joback Method
cpg	1657.68	J/mol×K	1360.55	Joback Method
cpg	1667.62	J/mol×K	1406.24	Joback Method
dvisc	0.0000922	Pa×s	667.25	Joback Method
dvisc	0.0000471	Pa×s	744.73	Joback Method

dvisc	0.0000273	Pa×s	822.20	Joback Method
dvisc	0.0000174	Pa×s	899.67	Joback Method
dvisc	0.0000119	Pa×s	977.15	Joback Method
dvisc	0.0000086	Pa×s	1054.62	Joback Method
dvisc	0.0000065	Pa×s	1132.10	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=U369926&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