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

Inchi: InChI=1S/C30H49ClO4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-20-23-34-28(32)30(6-2

InchiKey: RMKQHZOHCVNPCL-UHFFFAOYSA-N

Formula: C30H49ClO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1

Mol. weight [g/mol]: 509.16

Physical Properties

Property code	Value	Unit	Source
gf	-182.06	kJ/mol	Joback Method
hf	-963.03	kJ/mol	Joback Method
hfus	69.08	kJ/mol	Joback Method
hvap	107.38	kJ/mol	Joback Method
log10ws	-10.36		Crippen Method
logp	9.385		Crippen Method
mcvol	436.920	ml/mol	McGowan Method
pc	721.46	kPa	Joback Method
rinpol	3344.00		NIST Webbook
rinpol	3344.00		NIST Webbook
tb	1109.22	K	Joback Method
tc	1371.45	K	Joback Method
tf	655.98	K	Joback Method
vc	1.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1520.78	J/mol×K	1109.22	Joback Method
cpg	1538.59	J/mol×K	1152.92	Joback Method
cpg	1554.53	J/mol×K	1196.63	Joback Method
cpg	1568.75	J/mol×K	1240.33	Joback Method
cpg	1581.37	J/mol×K	1284.04	Joback Method
cpg	1592.55	J/mol×K	1327.74	Joback Method
cpg	1602.42	J/mol×K	1371.45	Joback Method
dvisc	0.0001060	Pa×s	655.98	Joback Method

dvisc	0.0000546	Pa×s	731.52	Joback Method
dvisc	0.0000318	Pa×s	807.06	Joback Method
dvisc	0.0000204	Pa×s	882.60	Joback Method
dvisc	0.0000140	Pa×s	958.14	Joback Method
dvisc	0.0000101	Pa×s	1033.68	Joback Method
dvisc	0.0000077	Pa×s	1109.22	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=U369925&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