Diethylmalonic acid, 4-chloro-2-methylphenyl pentadecyl ester

Inchi: InChI=1S/C29H47ClO4/c1-5-8-9-10-11-12-13-14-15-16-17-18-19-22-33-27(31)29(6-2,7-3

InchiKey: VBZSSUONBMGFDR-UHFFFAOYSA-N

Formula: C29H47ClO4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)cc1C

Mol. weight [g/mol]: 495.13

Physical Properties

Property code	Value	Unit	Source
gf	-190.48	kJ/mol	Joback Method
hf	-942.39	kJ/mol	Joback Method
hfus	66.49	kJ/mol	Joback Method
hvap	105.15	kJ/mol	Joback Method
log10ws	-9.94		Crippen Method
logp	8.995		Crippen Method
mcvol	422.830	ml/mol	McGowan Method
pc	760.16	kPa	Joback Method
rinpol	3277.00		NIST Webbook
rinpol	3277.00		NIST Webbook
tb	1086.34	K	Joback Method
tc	1338.15	K	Joback Method
tf	644.71	K	Joback Method
vc	1.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1457.32	J/mol×K	1086.34	Joback Method
cpg	1474.68	J/mol×K	1128.31	Joback Method
cpg	1490.30	J/mol×K	1170.28	Joback Method
cpg	1504.29	J/mol×K	1212.25	Joback Method
cpg	1516.78	J/mol×K	1254.21	Joback Method
cpg	1527.87	J/mol×K	1296.18	Joback Method
cpg	1537.70	J/mol×K	1338.15	Joback Method
dvisc	0.0001216	Pa×s	644.71	Joback Method

dvisc	0.0000632	Pa×s	718.32	Joback Method
dvisc	0.0000371	Pa×s	791.92	Joback Method
dvisc	0.0000238	Pa×s	865.52	Joback Method
dvisc	0.0000164	Pa×s	939.13	Joback Method
dvisc	0.0000119	Pa×s	1012.73	Joback Method
dvisc	0.0000090	Pa×s	1086.34	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=U370119&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