Diethylmalonic acid, 2-chloro-5-methylphenyl tridecyl ester

Inchi: InChI=1S/C27H43ClO4/c1-5-8-9-10-11-12-13-14-15-16-17-20-31-25(29)27(6-2,7-3)26(30

InchiKey: SIHDQJBQOOFFTB-UHFFFAOYSA-N

Formula: C27H43ClO4

SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 467.08

Physical Properties

Property code	Value	Unit	Source
gf	-207.32	kJ/mol	Joback Method
hf	-901.11	kJ/mol	Joback Method
hfus	61.31	kJ/mol	Joback Method
hvap	100.70	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.214		Crippen Method
mcvol	394.650	ml/mol	McGowan Method
pc	847.51	kPa	Joback Method
rinpol	3048.00		NIST Webbook
rinpol	3048.00		NIST Webbook
tb	1040.58	K	Joback Method
tc	1275.64	K	Joback Method
tf	622.17	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1331.37	J/mol×K	1040.58	Joback Method
cpg	1399.91	J/mol×K	1236.47	Joback Method
cpg	1388.93	J/mol×K	1197.29	Joback Method
cpg	1376.67	J/mol×K	1158.11	Joback Method
cpg	1363.05	J/mol×K	1118.93	Joback Method
cpg	1347.98	J/mol×K	1079.76	Joback Method
cpg	1409.70	J/mol×K	1275.64	Joback Method
dvisc	0.0000125	Pa×s	1040.58	Joback Method

dvisc	0.0000164	Pa×s	970.84	Joback Method
dvisc	0.0000225	Pa×s	901.11	Joback Method
dvisc	0.0000324	Pa×s	831.38	Joback Method
dvisc	0.0000500	Pa×s	761.64	Joback Method
dvisc	0.0000841	Pa×s	691.91	Joback Method
dvisc	0.0001590	Pa×s	622.17	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=U370462&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