Diethylmalonic acid, 2,4-dichloro-6-formylphenyl tridecyl ester

Inchi: InChI=1S/C27H40Cl2O5/c1-4-7-8-9-10-11-12-13-14-15-16-17-33-25(31)27(5-2,6-3)26(32

InchiKey: YBXPEPIFHUCPMQ-UHFFFAOYSA-N

Formula: C27H40Cl2O5

SMILES: CCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1C=O

Mol. weight [g/mol]: 515.51

Physical Properties

Property code	Value	Unit	Source
gf	-328.40	kJ/mol	Joback Method
hf	-1013.90	kJ/mol	Joback Method
hfus	67.40	kJ/mol	Joback Method
hvap	112.46	kJ/mol	Joback Method
log10ws	-9.55		Crippen Method
logp	8.372		Crippen Method
mcvol	408.460	ml/mol	McGowan Method
pc	858.47	kPa	Joback Method
rinpol	3296.00		NIST Webbook
rinpol	3296.00		NIST Webbook
tb	1131.65	K	Joback Method
tc	1394.61	K	Joback Method
tf	706.61	K	Joback Method
vc	1.591	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1360.31	J/mol×K	1131.65	Joback Method
cpg	1373.80	J/mol×K	1175.48	Joback Method
cpg	1385.59	J/mol×K	1219.30	Joback Method
cpg	1395.79	J/mol×K	1263.13	Joback Method
cpg	1404.52	J/mol×K	1306.95	Joback Method
cpg	1411.89	J/mol×K	1350.78	Joback Method
cpg	1418.01	J/mol×K	1394.61	Joback Method
dvisc	0.0001057	Pa×s	706.61	Joback Method

dvisc	0.0000612	Pa×s	777.45	Joback Method
dvisc	0.0000388	Pa×s	848.29	Joback Method
dvisc	0.0000264	Pa×s	919.13	Joback Method
dvisc	0.0000189	Pa×s	989.97	Joback Method
dvisc	0.0000142	Pa×s	1060.81	Joback Method
dvisc	0.0000111	Pa×s	1131.65	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=U370073&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