Diethylmalonic acid, 2-chlorophenyl octadecyl ester

Inchi: InChI=1S/C31H51ClO4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-20-23-26-35-29(33)3

InchiKey: ZQRPUCLRIFRTRS-UHFFFAOYSA-N

Formula: C31H51ClO4

SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1Cl

Mol. weight [g/mol]: 523.19

Physical Properties

Property code	Value	Unit	Source
gf	-164.01	kJ/mol	Joback Method
hf	-972.20	kJ/mol	Joback Method
hfus	72.05	kJ/mol	Joback Method
hvap	108.94	kJ/mol	Joback Method
log10ws	-10.72		Crippen Method
logp	9.856		Crippen Method
mcvol	451.010	ml/mol	McGowan Method
pc	691.07	kPa	Joback Method
rinpol	3511.00		NIST Webbook
rinpol	3511.00		NIST Webbook
tb	1127.12	K	Joback Method
tc	1399.57	K	Joback Method
tf	654.73	K	Joback Method
vc	1.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.63	J/mol×K	1127.12	Joback Method
cpg	1604.25	J/mol×K	1172.53	Joback Method
cpg	1620.95	J/mol×K	1217.94	Joback Method
cpg	1635.92	J/mol×K	1263.34	Joback Method
cpg	1649.32	J/mol×K	1308.75	Joback Method
cpg	1661.34	J/mol×K	1354.16	Joback Method
cpg	1672.14	J/mol×K	1399.57	Joback Method
dvisc	0.0001027	Pa×s	654.73	Joback Method

dvisc	0.0000502	Pa×s	733.46	Joback Method
dvisc	0.0000282	Pa×s	812.19	Joback Method
dvisc	0.0000176	Pa×s	890.92	Joback Method
dvisc	0.0000118	Pa×s	969.66	Joback Method
dvisc	0.0000084	Pa×s	1048.39	Joback Method
dvisc	0.0000063	Pa×s	1127.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369628&Units=SI
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

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

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