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

Inchi: InChI=1S/C28H45ClO4/c1-5-8-9-10-11-12-13-14-15-16-17-18-21-32-26(30)28(6-2,7-3)27

InchiKey: LVCZQCJVEWODPZ-UHFFFAOYSA-N

Formula: C28H45ClO4

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

Mol. weight [g/mol]: 481.11

Physical Properties

Property code	Value	Unit	Source
gf	-198.90	kJ/mol	Joback Method
hf	-921.75	kJ/mol	Joback Method
hfus	63.90	kJ/mol	Joback Method
hvap	102.92	kJ/mol	Joback Method
log10ws	-9.52		Crippen Method
logp	8.605		Crippen Method
mcvol	408.740	ml/mol	McGowan Method
pc	802.06	kPa	Joback Method
rinpol	3148.00		NIST Webbook
rinpol	3148.00		NIST Webbook
tb	1063.46	K	Joback Method
tc	1306.25	K	Joback Method
tf	633.44	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1394.17	J/mol×K	1063.46	Joback Method
cpg	1411.13	J/mol×K	1103.92	Joback Method
cpg	1426.46	J/mol×K	1144.39	Joback Method
cpg	1440.26	J/mol×K	1184.85	Joback Method
cpg	1452.62	J/mol×K	1225.32	Joback Method
cpg	1463.66	J/mol×K	1265.78	Joback Method
cpg	1473.46	J/mol×K	1306.25	Joback Method
dvisc	0.0001392	Pa×s	633.44	Joback Method

dvisc	0.0000729	Pa×s	705.11	Joback Method
dvisc	0.0000431	Pa×s	776.78	Joback Method
dvisc	0.0000278	Pa×s	848.45	Joback Method
dvisc	0.0000192	Pa×s	920.12	Joback Method
dvisc	0.0000140	Pa×s	991.79	Joback Method
dvisc	0.0000107	Pa×s	1063.46	Joback Method

Sources

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=U370463&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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