Diethylmalonic acid, tetradecyl 2,3,5-trichlorophenyl ester

Inchi: InChI=1S/C27H41Cl3O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-33-25(31)27(5-2,6-3)26

InchiKey: CEODCIMUVFQOQN-UHFFFAOYSA-N

Formula: C27H41Cl3O4

SMILES: CCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1Cl

Mol. weight [g/mol]: 535.97

Physical Properties

Property code	Value	Unit	Source
gf	-240.81	kJ/mol	Joback Method
hf	-944.06	kJ/mol	Joback Method
hfus	69.31	kJ/mol	Joback Method
hvap	110.13	kJ/mol	Joback Method
log10ws	-10.41		Crippen Method
logp	9.603		Crippen Method
mcvol	419.130	ml/mol	McGowan Method
pc	805.25	kPa	Joback Method
rinpol	3324.00		NIST Webbook
rinpol	3324.00		NIST Webbook
tb	1120.42	K	Joback Method
tc	1378.77	K	Joback Method
tf	694.53	K	Joback Method
vc	1.623	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1375.46	J/mol×K	1120.42	Joback Method
cpg	1389.74	J/mol×K	1163.48	Joback Method
cpg	1402.39	J/mol×K	1206.54	Joback Method
cpg	1413.53	J/mol×K	1249.60	Joback Method
cpg	1423.26	J/mol×K	1292.66	Joback Method
cpg	1431.70	J/mol×K	1335.72	Joback Method
cpg	1438.97	J/mol×K	1378.77	Joback Method
dvisc	0.0000877	Pa×s	694.53	Joback Method

dvisc	0.0000499	Pa×s	765.51	Joback Method
dvisc	0.0000312	Pa×s	836.49	Joback Method
dvisc	0.0000210	Pa×s	907.48	Joback Method
dvisc	0.0000150	Pa×s	978.46	Joback Method
dvisc	0.0000112	Pa×s	1049.44	Joback Method
dvisc	0.0000087	Pa×s	1120.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370555&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