Diethylmalonic acid, 2,6-dichlorophenyl pentadecyl ester

Inchi: InChI=1S/C28H44Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-22-33-26(31)28(5-2,6-3
InchiKey: ZXJZNBYJQWVLIP-UHFFFAOYSA-N
Formula: C28H44Cl2O4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 515.55

Physical Properties

Property code	Value	Unit	Source
gf	-210.83	kJ/mol	Joback Method
hf	-937.49	kJ/mol	Joback Method
hfus	68.09	kJ/mol	Joback Method
hvap	107.31	kJ/mol	Joback Method
log10ws	-10.15		Crippen Method
logp	9.340		Crippen Method
mcvol	420.980	ml/mol	McGowan Method
pc	785.51	kPa	Joback Method
rinpol	3326.00		NIST Webbook
rinpol	3326.00		NIST Webbook
tb	1100.89	K	Joback Method
tc	1355.25	K	Joback Method
tf	663.36	K	Joback Method
vc	1.631	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1417.56	J/mol×K	1100.89	Joback Method
cpg	1481.94	J/mol×K	1312.85	Joback Method
cpg	1471.88	J/mol×K	1270.46	Joback Method
cpg	1460.54	J/mol×K	1228.07	Joback Method
cpg	1447.78	J/mol×K	1185.68	Joback Method
cpg	1433.49	J/mol×K	1143.28	Joback Method
cpg	1490.83	J/mol×K	1355.25	Joback Method
dvisc	0.0000087	Pa×s	1100.89	Joback Method

dvisc	0.0000115	Pa×s	1027.97	Joback Method
dvisc	0.0000156	Pa×s	955.05	Joback Method
dvisc	0.0000225	Pa×s	882.12	Joback Method
dvisc	0.0000345	Pa×s	809.20	Joback Method
dvisc	0.0000577	Pa×s	736.28	Joback Method
dvisc	0.0001080	Pa×s	663.36	Joback Method

Sources

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=U369942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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