Dimethylmalonic acid, pentadecyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C26H39Cl3O4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-17-32-24(30)26(2,3)25(31

InchiKey: DLKNKPYNAPLIPH-UHFFFAOYSA-N

Formula: C26H39Cl3O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)(C)C(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 521.94

Physical Properties

Property code	Value	Unit	Source
gf	-249.23	kJ/mol	Joback Method
hf	-923.42	kJ/mol	Joback Method
hfus	66.72	kJ/mol	Joback Method
hvap	107.90	kJ/mol	Joback Method
log10ws	-10.00		Crippen Method
logp	9.213		Crippen Method
mcvol	405.040	ml/mol	McGowan Method
pc	850.98	kPa	Joback Method
rinpol	3280.00		NIST Webbook
tb	1097.54	K	Joback Method
tc	1347.16	K	Joback Method
tf	683.26	K	Joback Method
vc	1.567	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1313.61	J/mol×K	1097.54	Joback Method
cpg	1327.57	J/mol×K	1139.14	Joback Method
cpg	1339.99	J/mol×K	1180.75	Joback Method
cpg	1350.98	J/mol×K	1222.35	Joback Method
cpg	1360.64	J/mol×K	1263.95	Joback Method
cpg	1369.05	J/mol×K	1305.55	Joback Method
cpg	1376.31	J/mol×K	1347.16	Joback Method
dvisc	0.0001003	Pa×s	683.26	Joback Method
dvisc	0.0000576	Pa×s	752.31	Joback Method

dvisc	0.0000363	Pa×s	821.35	Joback Method
dvisc	0.0000246	Pa×s	890.40	Joback Method
dvisc	0.0000176	Pa×s	959.45	Joback Method
dvisc	0.0000132	Pa×s	1028.49	Joback Method
dvisc	0.0000103	Pa×s	1097.54	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=U363657&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