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

Inchi: InChI=1S/C25H37Cl3O4/c1-4-7-8-9-10-11-12-13-14-15-16-31-23(29)25(5-2,6-3)24(30)32
InchiKey: ZMIQNJWSFDDUDR-UHFFFAOYSA-N
Formula: C25H37Cl3O4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]: 507.92

Physical Properties

Property code	Value	Unit	Source
gf	-257.65	kJ/mol	Joback Method
hf	-902.78	kJ/mol	Joback Method
hfus	64.13	kJ/mol	Joback Method
hvap	105.68	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	8.823		Crippen Method
mcvol	390.950	ml/mol	McGowan Method
pc	900.72	kPa	Joback Method
rinpol	3118.00		NIST Webbook
rinpol	3118.00		NIST Webbook
tb	1074.66	K	Joback Method
tc	1316.85	K	Joback Method
tf	671.99	K	Joback Method
vc	1.512	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1252.13	J/mol×K	1074.66	Joback Method
cpg	1265.79	J/mol×K	1115.03	Joback Method
cpg	1278.01	J/mol×K	1155.39	Joback Method
cpg	1288.87	J/mol×K	1195.76	Joback Method
cpg	1298.45	J/mol×K	1236.12	Joback Method
cpg	1306.83	J/mol×K	1276.49	Joback Method
cpg	1314.10	J/mol×K	1316.85	Joback Method
dvisc	0.0001146	Pa×s	671.99	Joback Method

dvisc	0.0000664	Pa×s	739.10	Joback Method
dvisc	0.0000422	Pa×s	806.21	Joback Method
dvisc	0.0000287	Pa×s	873.32	Joback Method
dvisc	0.0000206	Pa×s	940.44	Joback Method
dvisc	0.0000155	Pa×s	1007.55	Joback Method
dvisc	0.0000121	Pa×s	1074.66	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=U370554&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