Diethylmalonic acid, 3,5-dichlorophenyl dodecyl ester

Inchi: InChI=1S/C25H38Cl2O4/c1-4-7-8-9-10-11-12-13-14-15-16-30-23(28)25(5-2,6-3)24(29)31
InchiKey: CWJBGSDVAHUZPK-UHFFFAOYSA-N
Formula: C25H38Cl2O4
SMILES: CCCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]: 473.47

Physical Properties

Property code	Value	Unit	Source
gf	-236.09	kJ/mol	Joback Method
hf	-875.57	kJ/mol	Joback Method
hfus	60.32	kJ/mol	Joback Method
hvap	100.63	kJ/mol	Joback Method
log10ws	-8.89		Crippen Method
logp	8.169		Crippen Method
mcvol	378.710	ml/mol	McGowan Method
pc	929.51	kPa	Joback Method
rinpol	2935.00		NIST Webbook
rinpol	2935.00		NIST Webbook
tb	1032.25	K	Joback Method
tc	1263.93	K	Joback Method
tf	629.55	K	Joback Method
vc	1.462	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1231.13	J/mol×K	1032.25	Joback Method
cpg	1246.05	J/mol×K	1070.86	Joback Method
cpg	1259.58	J/mol×K	1109.48	Joback Method
cpg	1271.80	J/mol×K	1148.09	Joback Method
cpg	1282.79	J/mol×K	1186.70	Joback Method
cpg	1292.61	J/mol×K	1225.31	Joback Method
cpg	1301.36	J/mol×K	1263.93	Joback Method
dvisc	0.0001617	Pa×s	629.55	Joback Method

dvisc	0.0000888	Pa×s	696.67	Joback Method
dvisc	0.0000542	Pa×s	763.78	Joback Method
dvisc	0.0000358	Pa×s	830.90	Joback Method
dvisc	0.0000252	Pa×s	898.02	Joback Method
dvisc	0.0000186	Pa×s	965.13	Joback Method
dvisc	0.0000143	Pa×s	1032.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370446&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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