Diethylmalonic acid, 2,4,5-trichlorophenyl undecyl ester

Inchi: InChI=1S/C24H35Cl3O4/c1-4-7-8-9-10-11-12-13-14-15-30-22(28)24(5-2,6-3)23(29)31-21
InchiKey: FGOIWICXRNEDSC-UHFFFAOYSA-N
Formula: C24H35Cl3O4
SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 493.89

Physical Properties

Property code	Value	Unit	Source
gf	-266.07	kJ/mol	Joback Method
hf	-882.14	kJ/mol	Joback Method
hfus	61.54	kJ/mol	Joback Method
hvap	103.45	kJ/mol	Joback Method
log10ws	-9.16		Crippen Method
logp	8.433		Crippen Method
mcvol	376.860	ml/mol	McGowan Method
pc	954.96	kPa	Joback Method
rinpol	3042.00		NIST Webbook
rinpol	3042.00		NIST Webbook
tb	1051.78	K	Joback Method
tc	1287.77	K	Joback Method
tf	660.72	K	Joback Method
vc	1.456	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.03	J/mol×K	1051.78	Joback Method
cpg	1204.44	J/mol×K	1091.11	Joback Method
cpg	1216.47	J/mol×K	1130.44	Joback Method
cpg	1227.20	J/mol×K	1169.78	Joback Method
cpg	1236.71	J/mol×K	1209.11	Joback Method
cpg	1245.07	J/mol×K	1248.44	Joback Method
cpg	1252.34	J/mol×K	1287.77	Joback Method
dvisc	0.0001306	Pa×s	660.72	Joback Method

dvisc	0.0000765	Pa×s	725.90	Joback Method
dvisc	0.0000489	Pa×s	791.07	Joback Method
dvisc	0.0000335	Pa×s	856.25	Joback Method
dvisc	0.0000242	Pa×s	921.43	Joback Method
dvisc	0.0000182	Pa×s	986.60	Joback Method
dvisc	0.0000142	Pa×s	1051.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370538&Units=SI

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

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