Diethylmalonic acid, 2,4-dichloro-6-formylphenyl undecyl ester

Inchi: InChI=1S/C25H36Cl2O5/c1-4-7-8-9-10-11-12-13-14-15-31-23(29)25(5-2,6-3)24(30)32-22

InchiKey: YGYFSIXYRYTRHU-UHFFFAOYSA-N

Formula: C25H36Cl2O5

SMILES: CCCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1C=O

Mol. weight [g/mol]: 487.46

Physical Properties

Property code	Value	Unit	Source
gf	-345.24	kJ/mol	Joback Method
hf	-972.62	kJ/mol	Joback Method
hfus	62.22	kJ/mol	Joback Method
hvap	108.01	kJ/mol	Joback Method
log10ws	-8.72		Crippen Method
logp	7.592		Crippen Method
mcvol	380.280	ml/mol	McGowan Method
pc	963.87	kPa	Joback Method
rinpol	3101.00		NIST Webbook
rinpol	3101.00		NIST Webbook
tb	1085.89	K	Joback Method
tc	1331.48	K	Joback Method
tf	684.07	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1237.61	J/mol×K	1085.89	Joback Method
cpg	1288.08	J/mol×K	1290.55	Joback Method
cpg	1280.65	J/mol×K	1249.61	Joback Method
cpg	1271.97	J/mol×K	1208.68	Joback Method
cpg	1261.96	J/mol×K	1167.75	Joback Method
cpg	1250.53	J/mol×K	1126.82	Joback Method
cpg	1294.35	J/mol×K	1331.48	Joback Method
dvisc	0.0000154	Pa×s	1085.89	Joback Method

dvisc	0.0000196	Pa×s	1018.92	Joback Method
dvisc	0.0000260	Pa×s	951.95	Joback Method
dvisc	0.0000359	Pa×s	884.98	Joback Method
dvisc	0.0000522	Pa×s	818.01	Joback Method
dvisc	0.0000812	Pa×s	751.04	Joback Method
dvisc	0.0001378	Pa×s	684.07	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=U370071&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