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

Inchi: InChI=1S/C23H32Cl2O5/c1-4-7-8-9-10-11-12-13-29-21(27)23(5-2,6-3)22(28)30-20-17(16
InchiKey: AXTIEIAQPMBBPJ-UHFFFAOYSA-N
Formula: C23H32Cl2O5
SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1C=O
Mol. weight [g/mol]: 459.40

Physical Properties

Property code	Value	Unit	Source
gf	-362.08	kJ/mol	Joback Method
hf	-931.34	kJ/mol	Joback Method
hfus	57.04	kJ/mol	Joback Method
hvap	103.56	kJ/mol	Joback Method
log10ws	-7.88		Crippen Method
logp	6.811		Crippen Method
mcvol	352.100	ml/mol	McGowan Method
pc	1089.94	kPa	Joback Method
rinpol	2886.00		NIST Webbook
rinpol	2886.00		NIST Webbook
tb	1040.13	K	Joback Method
tc	1273.42	K	Joback Method
tf	661.53	K	Joback Method
vc	1.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.42	J/mol×K	1040.13	Joback Method
cpg	1165.90	J/mol×K	1234.54	Joback Method
cpg	1158.43	J/mol×K	1195.66	Joback Method
cpg	1149.81	J/mol×K	1156.77	Joback Method
cpg	1139.98	J/mol×K	1117.89	Joback Method
cpg	1128.86	J/mol×K	1079.01	Joback Method
cpg	1172.27	J/mol×K	1273.42	Joback Method
dvisc	0.0000212	Pa×s	1040.13	Joback Method

dvisc	0.0000269	Pa×s	977.03	Joback Method
dvisc	0.0000354	Pa×s	913.93	Joback Method
dvisc	0.0000485	Pa×s	850.83	Joback Method
dvisc	0.0000698	Pa×s	787.73	Joback Method
dvisc	0.0001070	Pa×s	724.63	Joback Method
dvisc	0.0001780	Pa×s	661.53	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=U370069&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