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

Inchi: InChI=1S/C26H38Cl2O5/c1-4-7-8-9-10-11-12-13-14-15-16-32-24(30)26(5-2,6-3)25(31)33

InchiKey: JQGOSOMUUOQLOX-UHFFFAOYSA-N

Formula: C26H38Cl2O5

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

Mol. weight [g/mol]: 501.48

Physical Properties

Property code	Value	Unit	Source
gf	-336.82	kJ/mol	Joback Method
hf	-993.26	kJ/mol	Joback Method
hfus	64.81	kJ/mol	Joback Method
hvap	110.24	kJ/mol	Joback Method
log10ws	-9.13		Crippen Method
logp	7.982		Crippen Method
mcvol	394.370	ml/mol	McGowan Method
pc	908.89	kPa	Joback Method
rinpol	3199.00		NIST Webbook
tb	1108.77	K	Joback Method
tc	1362.36	K	Joback Method
tf	695.34	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1298.79	J/mol×K	1108.77	Joback Method
cpg	1311.98	J/mol×K	1151.04	Joback Method
cpg	1323.58	J/mol×K	1193.30	Joback Method
cpg	1333.68	J/mol×K	1235.57	Joback Method
cpg	1342.39	J/mol×K	1277.83	Joback Method
cpg	1349.79	J/mol×K	1320.10	Joback Method
cpg	1355.99	J/mol×K	1362.36	Joback Method
dvisc	0.0001208	Pa×s	695.34	Joback Method
dvisc	0.0000705	Pa×s	764.25	Joback Method

dvisc	0.0000450	Pa×s	833.15	Joback Method
dvisc	0.0000308	Pa×s	902.06	Joback Method
dvisc	0.0000222	Pa×s	970.96	Joback Method
dvisc	0.0000167	Pa×s	1039.87	Joback Method
dvisc	0.0000130	Pa×s	1108.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370072&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