Dimethylmalonic acid, 2,4-dichloro-6-formylphenyl isohexyl ester

Inchi: InChI=1S/C18H22Cl2O5/c1-11(2)6-5-7-24-16(22)18(3,4)17(23)25-15-12(10-21)8-13(19)9

InchiKey: YMQHVEFOVRHIHC-UHFFFAOYSA-N

Formula: C18H22Cl2O5

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

Mol. weight [g/mol]: 389.27

Physical Properties

Property code	Value	Unit	Source
gf	-406.62	kJ/mol	Joback Method
hf	-833.42	kJ/mol	Joback Method
hfus	40.57	kJ/mol	Joback Method
hvap	92.04	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.717		Crippen Method
mcvol	281.650	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	2391.00		NIST Webbook
rinpol	2391.00		NIST Webbook
tb	925.29	K	Joback Method
tc	1148.08	K	Joback Method
tf	590.18	K	Joback Method
vc	1.081	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	822.68	J/mol×K	925.29	Joback Method
cpg	834.18	J/mol×K	962.42	Joback Method
cpg	844.56	J/mol×K	999.55	Joback Method
cpg	853.86	J/mol×K	1036.68	Joback Method
cpg	862.09	J/mol×K	1073.81	Joback Method
cpg	869.31	J/mol×K	1110.94	Joback Method
cpg	875.55	J/mol×K	1148.08	Joback Method
dvisc	0.0003473	Pa×s	590.18	Joback Method

dvisc	0.0002100	Pa×s	646.03	Joback Method
dvisc	0.0001375	Pa×s	701.88	Joback Method
dvisc	0.0000959	Pa×s	757.74	Joback Method
dvisc	0.0000702	Pa×s	813.59	Joback Method
dvisc	0.0000536	Pa×s	869.44	Joback Method
dvisc	0.0000422	Pa×s	925.29	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=U363634&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