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

Inchi: InChI=1S/C17H20Cl2O5/c1-4-7-23-15(21)17(5-2,6-3)16(22)24-14-11(10-20)8-12(18)9-13

InchiKey: NMRCKKZDBLSAAF-UHFFFAOYSA-N

Formula: C17H20Cl2O5

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

Mol. weight [g/mol]: 375.24

Physical Properties

Property code	Value	Unit	Source
gf	-412.60	kJ/mol	Joback Method
hf	-807.50	kJ/mol	Joback Method
hfus	41.50	kJ/mol	Joback Method
hvap	90.20	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.471		Crippen Method
mcvol	267.560	ml/mol	McGowan Method
pc	1661.90	kPa	Joback Method
rinpol	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
tb	902.85	K	Joback Method
tc	1123.79	K	Joback Method
tf	593.91	K	Joback Method
vc	1.032	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.21	J/mol×K	902.85	Joback Method
cpg	776.43	J/mol×K	939.67	Joback Method
cpg	786.60	J/mol×K	976.50	Joback Method
cpg	795.74	J/mol×K	1013.32	Joback Method
cpg	803.89	J/mol×K	1050.14	Joback Method
cpg	811.07	J/mol×K	1086.97	Joback Method
cpg	817.32	J/mol×K	1123.79	Joback Method
dvisc	0.0003606	Pa×s	593.91	Joback Method

dvisc	0.0002314	Pa×s	645.40	Joback Method
dvisc	0.0001585	Pa×s	696.89	Joback Method
dvisc	0.0001144	Pa×s	748.38	Joback Method
dvisc	0.0000861	Pa×s	799.87	Joback Method
dvisc	0.0000671	Pa×s	851.36	Joback Method
dvisc	0.0000538	Pa×s	902.85	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=U370062&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