Dimethylmalonic acid, di(2,4-dichloro-6-formylphenyl) ester

Inchi: InChI=1S/C19H12Cl4O6/c1-19(2,17(26)28-15-9(7-24)3-11(20)5-13(15)22)18(27)29-16-1
InchiKey: PNGYCDPOVQCQFZ-UHFFFAOYSA-N
Formula: C19H12Cl4O6
SMILES: CC(C)(C(=O)Oc1c(Cl)cc(Cl)cc1C=O)C(=O)Oc1c(Cl)cc(Cl)cc1C=O
Mol. weight [g/mol]: 478.11

Physical Properties

Property code	Value	Unit	Source
gf	-435.62	kJ/mol	Joback Method
hf	-763.72	kJ/mol	Joback Method
hfus	50.24	kJ/mol	Joback Method
hvap	114.41	kJ/mol	Joback Method
log10ws	-7.15		Crippen Method
logp	5.462		Crippen Method
mcvol	298.030	ml/mol	McGowan Method
pc	1796.98	kPa	Joback Method
rinpol	3173.00		NIST Webbook
tb	1113.75	K	Joback Method
tc	1372.50	K	Joback Method
tf	782.27	K	Joback Method
vc	1.151	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.49	J/mol×K	1113.75	Joback Method
cpg	796.61	J/mol×K	1156.87	Joback Method
cpg	799.51	J/mol×K	1200.00	Joback Method
cpg	801.23	J/mol×K	1243.12	Joback Method
cpg	801.82	J/mol×K	1286.25	Joback Method
cpg	801.32	J/mol×K	1329.37	Joback Method
cpg	799.77	J/mol×K	1372.50	Joback Method
dvisc	0.0001455	Pa×s	782.27	Joback Method
dvisc	0.0001046	Pa×s	837.52	Joback Method

dvisc	0.0000784	Pa×s	892.76	Joback Method
dvisc	0.0000608	Pa×s	948.01	Joback Method
dvisc	0.0000484	Pa×s	1003.26	Joback Method
dvisc	0.0000395	Pa×s	1058.50	Joback Method
dvisc	0.0000329	Pa×s	1113.75	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=U363641&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