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

Inchi: InChI=1S/C16H18Cl2O5/c1-9(2)8-22-14(20)16(3,4)15(21)23-13-10(7-19)5-11(17)6-12(13

InchiKey: MICXEHRGKOCCES-UHFFFAOYSA-N

Formula: C16H18Cl2O5

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

Mol. weight [g/mol]: 361.22

Physical Properties

Property code	Value	Unit	Source
gf	-423.46	kJ/mol	Joback Method
hf	-792.14	kJ/mol	Joback Method
hfus	35.39	kJ/mol	Joback Method
hvap	87.59	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.937		Crippen Method
mcvol	253.470	ml/mol	McGowan Method
pc	1812.32	kPa	Joback Method
rinpol	2203.00		NIST Webbook
rinpol	2203.00		NIST Webbook
tb	879.53	K	Joback Method
tc	1104.05	K	Joback Method
tf	567.64	K	Joback Method
vc	0.970	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	709.59	J/mol×K	879.53	Joback Method
cpg	754.64	J/mol×K	1066.63	Joback Method
cpg	747.64	J/mol×K	1029.21	Joback Method
cpg	739.67	J/mol×K	991.79	Joback Method
cpg	730.68	J/mol×K	954.37	Joback Method
cpg	720.67	J/mol×K	916.95	Joback Method
cpg	760.69	J/mol×K	1104.05	Joback Method
dvisc	0.0000571	Pa×s	879.53	Joback Method

dvisc	0.0000720	Pa×s	827.55	Joback Method
dvisc	0.0000936	Pa×s	775.57	Joback Method
dvisc	0.0001265	Pa×s	723.59	Joback Method
dvisc	0.0001790	Pa×s	671.60	Joback Method
dvisc	0.0002685	Pa×s	619.62	Joback Method
dvisc	0.0004339	Pa×s	567.64	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=U363631&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