Dimethylmalonic acid, 2,3-dichlorophenyl isobutyl ester

Inchi: InChI=1S/C15H18Cl2O4/c1-9(2)8-20-13(18)15(3,4)14(19)21-11-7-5-6-10(16)12(11)17/h5

InchiKey: RRZVLOVDSWMSGG-UHFFFAOYSA-N

Formula: C15H18Cl2O4

SMILES: CC(C)COC(=O)C(C)(C)C(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 333.21

Physical Properties

Property code	Value	Unit	Source
gf	-322.73	kJ/mol	Joback Method
hf	-674.45	kJ/mol	Joback Method
hfus	30.90	kJ/mol	Joback Method
hvap	77.98	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	4.124		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	2049.00		NIST Webbook
tb	803.01	K	Joback Method
tc	1026.59	K	Joback Method
tf	501.85	K	Joback Method
vc	0.896	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.84	J/mol×K	803.01	Joback Method
cpg	658.69	J/mol×K	840.27	Joback Method
cpg	670.48	J/mol×K	877.54	Joback Method
cpg	681.25	J/mol×K	914.80	Joback Method
cpg	691.01	J/mol×K	952.06	Joback Method
cpg	699.82	J/mol×K	989.33	Joback Method
cpg	707.70	J/mol×K	1026.59	Joback Method
dvisc	0.0005850	Pa×s	501.85	Joback Method
dvisc	0.0003390	Pa×s	552.04	Joback Method

dvisc	0.0002152	Pa×s	602.24	Joback Method
dvisc	0.0001465	Pa×s	652.43	Joback Method
dvisc	0.0001053	Pa×s	702.62	Joback Method
dvisc	0.0000791	Pa×s	752.82	Joback Method
dvisc	0.0000616	Pa×s	803.01	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=U363621&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