Dimethylmalonic acid, monochloride, 2-isopropoxyphenyl ester

Inchi: InChI=1S/C14H17ClO4/c1-9(2)18-10-7-5-6-8-11(10)19-13(17)14(3,4)12(15)16/h5-9H,1-4

InchiKey: WNTRJSMFKXIQBL-UHFFFAOYSA-N

Formula: C14H17ClO4

SMILES: CC(C)Oc1ccccc1OC(=O)C(C)(C)C(=O)Cl

Mol. weight [g/mol]: 284.74

Physical Properties

Property code	Value	Unit	Source
gf	-309.59	kJ/mol	Joback Method
hf	-626.60	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	70.71	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	3.171		Crippen Method
mcvol	211.480	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1611.00		NIST Webbook
rinpol	1611.00		NIST Webbook
tb	737.72	K	Joback Method
tc	960.89	K	Joback Method
tf	448.14	K	Joback Method
vc	0.791	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.01	J/mol×K	737.72	Joback Method
cpg	582.89	J/mol×K	774.92	Joback Method
cpg	595.70	J/mol×K	812.11	Joback Method
cpg	607.48	J/mol×K	849.31	Joback Method
cpg	618.27	J/mol×K	886.50	Joback Method
cpg	628.09	J/mol×K	923.70	Joback Method
cpg	636.97	J/mol×K	960.89	Joback Method
dvisc	0.0009482	Pa×s	448.14	Joback Method

dvisc	0.0005169	Pa×s	496.40	Joback Method
dvisc	0.0003137	Pa×s	544.67	Joback Method
dvisc	0.0002065	Pa×s	592.93	Joback Method
dvisc	0.0001448	Pa×s	641.19	Joback Method
dvisc	0.0001067	Pa×s	689.46	Joback Method
dvisc	0.0000818	Pa×s	737.72	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=U361867&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