Dimethylmalonic acid, 4-chlorophenyl isobutyl ester

Inchi: InChI=1S/C15H19ClO4/c1-10(2)9-19-13(17)15(3,4)14(18)20-12-7-5-11(16)6-8-12/h5-8,1

InchiKey: FIMZKLFPBAKZDH-UHFFFAOYSA-N

Formula: C15H19ClO4

SMILES: CC(C)COC(=O)C(C)(C)C(=O)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 298.76

Physical Properties

Property code	Value	Unit	Source
gf	-301.17	kJ/mol	Joback Method
hf	-647.24	kJ/mol	Joback Method
hfus	27.09	kJ/mol	Joback Method
hvap	72.94	kJ/mol	Joback Method
log10ws	-3.78		Crippen Method
logp	3.471		Crippen Method
mcvol	225.570	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	1866.00		NIST Webbook
rinpol	1866.00		NIST Webbook
tb	760.60	K	Joback Method
tc	980.46	K	Joback Method
tf	459.41	K	Joback Method
vc	0.848	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	622.79	J/mol×K	760.60	Joback Method
cpg	636.99	J/mol×K	797.24	Joback Method
cpg	650.11	J/mol×K	833.89	Joback Method
cpg	662.17	J/mol×K	870.53	Joback Method
cpg	673.23	J/mol×K	907.17	Joback Method
cpg	683.31	J/mol×K	943.82	Joback Method
cpg	692.44	J/mol×K	980.46	Joback Method
dvisc	0.0008588	Pa×s	459.41	Joback Method

dvisc	0.0004620	Pa×s	509.61	Joback Method
dvisc	0.0002778	Pa×s	559.81	Joback Method
dvisc	0.0001816	Pa×s	610.00	Joback Method
dvisc	0.0001267	Pa×s	660.20	Joback Method
dvisc	0.0000929	Pa×s	710.40	Joback Method
dvisc	0.0000711	Pa×s	760.60	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=U361972&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