Dimethylmalonic acid, 4-chlorophenyl propyl ester

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

InchiKey: UPJPDESZJDAAHC-UHFFFAOYSA-N

Formula: C14H17ClO4

SMILES: CCCOC(=O)C(C)(C)C(=O)Oc1ccc(Cl)cc1

Mol. weight [g/mol]: 284.74

Physical Properties

Property code	Value	Unit	Source
gf	-307.15	kJ/mol	Joback Method
hf	-621.32	kJ/mol	Joback Method
hfus	28.03	kJ/mol	Joback Method
hvap	71.10	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.225		Crippen Method
mcvol	211.480	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	1818.00		NIST Webbook
tb	738.16	K	Joback Method
tc	957.50	K	Joback Method
tf	463.14	K	Joback Method
vc	0.797	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	568.43	J/mol×K	738.16	Joback Method
cpg	582.06	J/mol×K	774.72	Joback Method
cpg	594.68	J/mol×K	811.27	Joback Method
cpg	606.30	J/mol×K	847.83	Joback Method
cpg	616.98	J/mol×K	884.39	Joback Method
cpg	626.73	J/mol×K	920.94	Joback Method
cpg	635.59	J/mol×K	957.50	Joback Method
dvisc	0.0008163	Pa×s	463.14	Joback Method
dvisc	0.0004774	Pa×s	508.98	Joback Method

dvisc	0.0003050	Pa×s	554.81	Joback Method
dvisc	0.0002087	Pa×s	600.65	Joback Method
dvisc	0.0001507	Pa×s	646.49	Joback Method
dvisc	0.0001136	Pa×s	692.32	Joback Method
dvisc	0.0000887	Pa×s	738.16	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=U361971&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