Dimethylmalonic acid, monochloride, 3-phenylpropyl ester

Inchi: InChI=1S/C14H17ClO3/c1-14(2,12(15)16)13(17)18-10-6-9-11-7-4-3-5-8-11/h3-5,7-8H,6,9

InchiKey: BMNDSPKXQWDZTK-UHFFFAOYSA-N

Formula: C14H17ClO3

SMILES: CC(C)(C(=O)Cl)C(=O)OCCCc1ccccc1

Mol. weight [g/mol]: 268.74

Physical Properties

Property code	Value	Unit	Source
gf	-192.52	kJ/mol	Joback Method
hf	-477.63	kJ/mol	Joback Method
hfus	27.23	kJ/mol	Joback Method
hvap	68.02	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.954		Crippen Method
mcvol	205.610	ml/mol	McGowan Method
pc	2183.60	kPa	Joback Method
rinpol	1798.00		NIST Webbook
tb	710.76	K	Joback Method
tc	931.73	K	Joback Method
tf	428.39	K	Joback Method
vc	0.779	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.60	J/mol×K	710.76	Joback Method
cpg	557.76	J/mol×K	747.59	Joback Method
cpg	570.86	J/mol×K	784.42	Joback Method
cpg	582.96	J/mol×K	821.24	Joback Method
cpg	594.12	J/mol×K	858.07	Joback Method
cpg	604.40	J/mol×K	894.90	Joback Method
cpg	613.84	J/mol×K	931.73	Joback Method
dvisc	0.0014179	Pa×s	428.39	Joback Method
dvisc	0.0007618	Pa×s	475.45	Joback Method

dvisc	0.0004578	Pa×s	522.51	Joback Method
dvisc	0.0002993	Pa×s	569.58	Joback Method
dvisc	0.0002087	Pa×s	616.64	Joback Method
dvisc	0.0001532	Pa×s	663.70	Joback Method
dvisc	0.0001172	Pa×s	710.76	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=U361848&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