Dimethylmalonic acid, monochloride, isohexyl ester

Inchi: InChI=1S/C11H19ClO3/c1-8(2)6-5-7-15-10(14)11(3,4)9(12)13/h8H,5-7H2,1-4H3
InchiKey: FWZMFPHPPPHGMC-UHFFFAOYSA-N
Formula: C11H19ClO3
SMILES: CC(C)CCCOC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]: 234.72

Physical Properties

Property code	Value	Unit	Source
gf	-332.63	kJ/mol	Joback Method
hf	-657.52	kJ/mol	Joback Method
hfus	21.89	kJ/mol	Joback Method
hvap	58.68	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.757		Crippen Method
mcvol	187.100	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	1358.00		NIST Webbook
tb	615.00	K	Joback Method
tc	811.61	K	Joback Method
tf	353.16	K	Joback Method
vc	0.714	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.26	J/mol×K	615.00	Joback Method
cpg	534.83	J/mol×K	778.84	Joback Method
cpg	523.62	J/mol×K	746.07	Joback Method
cpg	511.68	J/mol×K	713.30	Joback Method
cpg	498.99	J/mol×K	680.54	Joback Method
cpg	485.53	J/mol×K	647.77	Joback Method
cpg	545.35	J/mol×K	811.61	Joback Method
dvisc	0.0001660	Pa×s	615.00	Joback Method
dvisc	0.0002240	Pa×s	571.36	Joback Method

dvisc	0.0003175	Pa×s	527.72	Joback Method
dvisc	0.0004792	Pa×s	484.08	Joback Method
dvisc	0.0007849	Pa×s	440.44	Joback Method
dvisc	0.0014328	Pa×s	396.80	Joback Method
dvisc	0.0030351	Pa×s	353.16	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=U361729&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