Dimethylmalonic acid, monochloride, 2-methylpent-3-yl ester

Inchi: InChI=1S/C11H19ClO3/c1-6-8(7(2)3)15-10(14)11(4,5)9(12)13/h7-8H,6H2,1-5H3
InchiKey: FPLGPYWSBFFAOD-UHFFFAOYSA-N
Formula: C11H19ClO3
SMILES: CCC(OC(=O)C(C)(C)C(=O)Cl)C(C)C
Mol. weight [g/mol]: 234.72

Physical Properties

Property code	Value	Unit	Source
gf	-335.07	kJ/mol	Joback Method
hf	-662.80	kJ/mol	Joback Method
hfus	18.37	kJ/mol	Joback Method
hvap	58.30	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.756		Crippen Method
mcvol	187.100	ml/mol	McGowan Method
pc	2129.52	kPa	Joback Method
rinpol	1341.00		NIST Webbook
tb	614.56	K	Joback Method
tc	814.90	K	Joback Method
tf	338.16	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	471.70	J/mol×K	614.56	Joback Method
cpg	536.46	J/mol×K	781.51	Joback Method
cpg	525.08	J/mol×K	748.12	Joback Method
cpg	512.95	J/mol×K	714.73	Joback Method
cpg	500.02	J/mol×K	681.34	Joback Method
cpg	486.28	J/mol×K	647.95	Joback Method
cpg	547.11	J/mol×K	814.90	Joback Method
dvisc	0.0001549	Pa×s	614.56	Joback Method
dvisc	0.0002139	Pa×s	568.49	Joback Method

dvisc	0.0003126	Pa×s	522.43	Joback Method
dvisc	0.0004919	Pa×s	476.36	Joback Method
dvisc	0.0008527	Pa×s	430.29	Joback Method
dvisc	0.0016868	Pa×s	384.23	Joback Method
dvisc	0.0040182	Pa×s	338.16	Joback Method

Sources

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=U361805&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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