Dimethylmalonic acid, monochloride, 3-methylbutyl ester

Inchi: InChI=1S/C10H17ClO3/c1-7(2)5-6-14-9(13)10(3,4)8(11)12/h7H,5-6H2,1-4H3
InchiKey: IZBONMRVMDHJDM-UHFFFAOYSA-N
Formula: C10H17ClO3
SMILES: CC(C)CCOC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]: 220.69

Physical Properties

Property code	Value	Unit	Source
gf	-341.05	kJ/mol	Joback Method
hf	-636.88	kJ/mol	Joback Method
hfus	19.30	kJ/mol	Joback Method
hvap	56.46	kJ/mol	Joback Method
log10ws	-2.32		Crippen Method
logp	2.367		Crippen Method
mcvol	173.010	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	1246.00		NIST Webbook
rinpol	1246.00		NIST Webbook
tb	592.12	K	Joback Method
tc	791.38	K	Joback Method
tf	341.89	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.07	J/mol×K	592.12	Joback Method
cpg	435.71	J/mol×K	625.33	Joback Method
cpg	448.58	J/mol×K	658.54	Joback Method
cpg	460.71	J/mol×K	691.75	Joback Method
cpg	472.11	J/mol×K	724.96	Joback Method
cpg	482.81	J/mol×K	758.17	Joback Method
cpg	492.83	J/mol×K	791.38	Joback Method
dvisc	0.0033109	Pa×s	341.89	Joback Method

dvisc	0.0015851	Pa×s	383.59	Joback Method
dvisc	0.0008768	Pa×s	425.30	Joback Method
dvisc	0.0005391	Pa×s	467.00	Joback Method
dvisc	0.0003590	Pa×s	508.71	Joback Method
dvisc	0.0002543	Pa×s	550.41	Joback Method
dvisc	0.0001890	Pa×s	592.12	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=U361607&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