Dimethylmalonic acid, monochloride, octyl ester

Inchi: InChI=1S/C13H23ClO3/c1-4-5-6-7-8-9-10-17-12(16)13(2,3)11(14)15/h4-10H2,1-3H3
InchiKey: CNMCEFNYJFNGNI-UHFFFAOYSA-N
Formula: C13H23ClO3
SMILES: CCCCCCCCOC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]: 262.77

Physical Properties

Property code	Value	Unit	Source
gf	-313.35	kJ/mol	Joback Method
hf	-693.52	kJ/mol	Joback Method
hfus	30.59	kJ/mol	Joback Method
hvap	63.52	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.682		Crippen Method
mcvol	215.280	ml/mol	McGowan Method
pc	1772.85	kPa	Joback Method
rinpol	1598.00		NIST Webbook
tb	661.20	K	Joback Method
tc	850.26	K	Joback Method
tf	390.70	K	Joback Method
vc	0.832	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.58	J/mol×K	661.20	Joback Method
cpg	640.68	J/mol×K	818.75	Joback Method
cpg	628.78	J/mol×K	787.24	Joback Method
cpg	616.15	J/mol×K	755.73	Joback Method
cpg	602.76	J/mol×K	724.22	Joback Method
cpg	588.58	J/mol×K	692.71	Joback Method
cpg	651.87	J/mol×K	850.26	Joback Method
dvisc	0.0001363	Pa×s	661.20	Joback Method
dvisc	0.0001810	Pa×s	616.12	Joback Method

dvisc	0.0002512	Pa×s	571.03	Joback Method
dvisc	0.0003690	Pa×s	525.95	Joback Method
dvisc	0.0005825	Pa×s	480.87	Joback Method
dvisc	0.0010105	Pa×s	435.78	Joback Method
dvisc	0.0019909	Pa×s	390.70	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=U361683&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