Dimethylmalonic acid, monochloride, nonyl ester

Inchi: InChI=1S/C14H25ClO3/c1-4-5-6-7-8-9-10-11-18-13(17)14(2,3)12(15)16/h4-11H2,1-3H3
InchiKey: CICOLCJXMIRLLD-UHFFFAOYSA-N
Formula: C14H25ClO3
SMILES: CCCCCCCCCOC(=O)C(C)(C)C(=O)Cl
Mol. weight [g/mol]: 276.80

Physical Properties

Property code	Value	Unit	Source
gf	-304.93	kJ/mol	Joback Method
hf	-714.16	kJ/mol	Joback Method
hfus	33.18	kJ/mol	Joback Method
hvap	65.75	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.072		Crippen Method
mcvol	229.370	ml/mol	McGowan Method
pc	1637.78	kPa	Joback Method
rinpol	1697.00		NIST Webbook
tb	684.08	K	Joback Method
tc	871.70	K	Joback Method
tf	401.97	K	Joback Method
vc	0.887	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	626.98	J/mol×K	684.08	Joback Method
cpg	696.02	J/mol×K	840.43	Joback Method
cpg	683.78	J/mol×K	809.16	Joback Method
cpg	670.79	J/mol×K	777.89	Joback Method
cpg	657.01	J/mol×K	746.62	Joback Method
cpg	642.42	J/mol×K	715.35	Joback Method
cpg	707.54	J/mol×K	871.70	Joback Method
dvisc	0.0001186	Pa×s	684.08	Joback Method
dvisc	0.0001580	Pa×s	637.06	Joback Method

dvisc	0.0002202	Pa×s	590.04	Joback Method
dvisc	0.0003251	Pa×s	543.02	Joback Method
dvisc	0.0005168	Pa×s	496.01	Joback Method
dvisc	0.0009052	Pa×s	448.99	Joback Method
dvisc	0.0018077	Pa×s	401.97	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=U361711&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