Dimethylmalonic acid, monochloride, 4-octyl ester

Inchi: InChI=1S/C13H23ClO3/c1-5-7-9-10(8-6-2)17-12(16)13(3,4)11(14)15/h10H,5-9H2,1-4H3

InchiKey: KOACAVSGVBGTGN-UHFFFAOYSA-N

Formula: C13H23ClO3

SMILES: CCCCC(CCC)OC(=O)C(C)(C)C(=O)Cl

Mol. weight [g/mol]: 262.77

Physical Properties

Property code	Value	Unit	Source
gf	-315.79	kJ/mol	Joback Method
hf	-698.80	kJ/mol	Joback Method
hfus	27.07	kJ/mol	Joback Method
hvap	63.14	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.680		Crippen Method
mcvol	215.280	ml/mol	McGowan Method
pc	1784.86	kPa	Joback Method
rinpol	1477.00		NIST Webbook
tb	660.76	K	Joback Method
tc	852.92	K	Joback Method
tf	375.70	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.05	J/mol×K	660.76	Joback Method
cpg	642.21	J/mol×K	820.90	Joback Method
cpg	630.17	J/mol×K	788.87	Joback Method
cpg	617.36	J/mol×K	756.84	Joback Method
cpg	603.76	J/mol×K	724.81	Joback Method
cpg	589.33	J/mol×K	692.79	Joback Method
cpg	653.51	J/mol×K	852.92	Joback Method
dvisc	0.0001266	Pa×s	660.76	Joback Method
dvisc	0.0001716	Pa×s	613.25	Joback Method

dvisc	0.0002450	Pa×s	565.74	Joback Method
dvisc	0.0003733	Pa×s	518.23	Joback Method
dvisc	0.0006192	Pa×s	470.72	Joback Method
dvisc	0.0011508	Pa×s	423.21	Joback Method
dvisc	0.0025016	Pa×s	375.70	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=U361742&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