Malonic acid, 2-chloropropyl heptyl ester

Inchi: InChI=1S/C13H23ClO4/c1-3-4-5-6-7-8-17-12(15)9-13(16)18-10-11(2)14/h11H,3-10H2,1-
InchiKey: IEQDMFOGLIMBKT-UHFFFAOYSA-N
Formula: C13H23ClO4
SMILES: CCCCCCCOC(=O)CC(=O)OCC(C)Cl
Mol. weight [g/mol]: 278.77

Physical Properties

Property code	Value	Unit	Source
gf	-423.63	kJ/mol	Joback Method
hf	-822.27	kJ/mol	Joback Method
hfus	35.67	kJ/mol	Joback Method
hvap	66.84	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.061		Crippen Method
mcvol	221.150	ml/mol	McGowan Method
pc	1731.78	kPa	Joback Method
rinpol	1814.00		NIST Webbook
tb	686.41	K	Joback Method
tc	869.92	K	Joback Method
tf	395.51	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.84	J/mol×K	686.41	Joback Method
cpg	613.43	J/mol×K	716.99	Joback Method
cpg	627.27	J/mol×K	747.58	Joback Method
cpg	640.38	J/mol×K	778.16	Joback Method
cpg	652.76	J/mol×K	808.75	Joback Method
cpg	664.42	J/mol×K	839.33	Joback Method
cpg	675.35	J/mol×K	869.92	Joback Method
dvisc	0.0016130	Pa×s	395.51	Joback Method
dvisc	0.0008133	Pa×s	443.99	Joback Method

dvisc	0.0004693	Pa×s	492.48	Joback Method
dvisc	0.0002988	Pa×s	540.96	Joback Method
dvisc	0.0002049	Pa×s	589.44	Joback Method
dvisc	0.0001488	Pa×s	637.93	Joback Method
dvisc	0.0001131	Pa×s	686.41	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=U349029&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