Malonic acid, 2-chloropropyl ethyl ester

Inchi: InChI=1S/C8H13ClO4/c1-3-12-7(10)4-8(11)13-5-6(2)9/h6H,3-5H2,1-2H3
InchiKey: LNNJMHLJYAMEAG-UHFFFAOYSA-N
Formula: C8H13ClO4
SMILES: CCOC(=O)CC(=O)OCC(C)Cl
Mol. weight [g/mol]: 208.64

Physical Properties

Property code	Value	Unit	Source
gf	-465.73	kJ/mol	Joback Method
hf	-719.07	kJ/mol	Joback Method
hfus	22.72	kJ/mol	Joback Method
hvap	55.71	kJ/mol	Joback Method
log10ws	-1.16		Crippen Method
logp	1.110		Crippen Method
mcvol	150.700	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	1294.00		NIST Webbook
tb	572.01	K	Joback Method
tc	764.07	K	Joback Method
tf	339.16	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	348.36	J/mol×K	572.01	Joback Method
cpg	399.58	J/mol×K	732.06	Joback Method
cpg	390.35	J/mol×K	700.05	Joback Method
cpg	380.60	J/mol×K	668.04	Joback Method
cpg	370.35	J/mol×K	636.03	Joback Method
cpg	359.60	J/mol×K	604.02	Joback Method
cpg	408.30	J/mol×K	764.07	Joback Method
dvisc	0.0002071	Pa×s	572.01	Joback Method
dvisc	0.0002674	Pa×s	533.20	Joback Method

dvisc	0.0003594	Pa×s	494.39	Joback Method
dvisc	0.0005081	Pa×s	455.59	Joback Method
dvisc	0.0007662	Pa×s	416.78	Joback Method
dvisc	0.0012570	Pa×s	377.97	Joback Method
dvisc	0.0023096	Pa×s	339.16	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=U349026&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