Malonic acid, 2,2-dichloroethyl propyl ester

Inchi: InChI=1S/C8H12Cl2O4/c1-2-3-13-7(11)4-8(12)14-5-6(9)10/h6H,2-5H2,1H3
InchiKey: OSKMQXOYMHLDJW-UHFFFAOYSA-N
Formula: C8H12Cl2O4
SMILES: CCCOC(=O)CC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 243.08

Physical Properties

Property code	Value	Unit	Source
gf	-477.66	kJ/mol	Joback Method
hf	-734.81	kJ/mol	Joback Method
hfus	26.92	kJ/mol	Joback Method
hvap	60.10	kJ/mol	Joback Method
log10ws	-1.81		Crippen Method
logp	1.677		Crippen Method
mcvol	162.940	ml/mol	McGowan Method
pc	2603.08	kPa	Joback Method
rinpol	1470.00		NIST Webbook
rinpol	1470.00		NIST Webbook
tb	609.44	K	Joback Method
tc	805.72	K	Joback Method
tf	369.08	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.93	J/mol×K	609.44	Joback Method
cpg	420.74	J/mol×K	773.01	Joback Method
cpg	412.26	J/mol×K	740.30	Joback Method
cpg	403.23	J/mol×K	707.58	Joback Method
cpg	393.66	J/mol×K	674.87	Joback Method
cpg	383.56	J/mol×K	642.15	Joback Method
cpg	428.67	J/mol×K	805.72	Joback Method
dvisc	0.0001919	Pa×s	609.44	Joback Method

dvisc	0.0002469	Pa×s	569.38	Joback Method
dvisc	0.0003299	Pa×s	529.32	Joback Method
dvisc	0.0004623	Pa×s	489.26	Joback Method
dvisc	0.0006879	Pa×s	449.20	Joback Method
dvisc	0.0011065	Pa×s	409.14	Joback Method
dvisc	0.0019734	Pa×s	369.08	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=U349059&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