Malonic acid, 2-chloropropyl hexyl ester

Inchi: InChI=1S/C12H21ClO4/c1-3-4-5-6-7-16-11(14)8-12(15)17-9-10(2)13/h10H,3-9H2,1-2H3
InchiKey: XHGYTOCDBVKYCB-UHFFFAOYSA-N
Formula: C12H21ClO4
SMILES: CCCCCCOC(=O)CC(=O)OCC(C)Cl
Mol. weight [g/mol]: 264.75

Physical Properties

Property code	Value	Unit	Source
gf	-432.05	kJ/mol	Joback Method
hf	-801.63	kJ/mol	Joback Method
hfus	33.08	kJ/mol	Joback Method
hvap	64.62	kJ/mol	Joback Method
log10ws	-2.84		Crippen Method
logp	2.671		Crippen Method
mcvol	207.060	ml/mol	McGowan Method
pc	1878.90	kPa	Joback Method
rinpol	1722.00		NIST Webbook
tb	663.53	K	Joback Method
tc	848.07	K	Joback Method
tf	384.24	K	Joback Method
vc	0.798	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.79	J/mol×K	663.53	Joback Method
cpg	559.86	J/mol×K	694.29	Joback Method
cpg	573.23	J/mol×K	725.04	Joback Method
cpg	585.92	J/mol×K	755.80	Joback Method
cpg	597.91	J/mol×K	786.56	Joback Method
cpg	609.21	J/mol×K	817.32	Joback Method
cpg	619.82	J/mol×K	848.07	Joback Method
dvisc	0.0017583	Pa×s	384.24	Joback Method
dvisc	0.0008988	Pa×s	430.79	Joback Method

dvisc	0.0005237	Pa×s	477.34	Joback Method
dvisc	0.0003359	Pa×s	523.88	Joback Method
dvisc	0.0002316	Pa×s	570.43	Joback Method
dvisc	0.0001690	Pa×s	616.98	Joback Method
dvisc	0.0001288	Pa×s	663.53	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U349028&Units=SI

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

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