Malonic acid, 2-chloropropyl nonyl ester

Inchi: InChI=1S/C15H27ClO4/c1-3-4-5-6-7-8-9-10-19-14(17)11-15(18)20-12-13(2)16/h13H,3-12
InchiKey: VVUNFCIBQWZLJJ-UHFFFAOYSA-N
Formula: C15H27ClO4
SMILES: CCCCCCCCCOC(=O)CC(=O)OCC(C)Cl
Mol. weight [g/mol]: 306.82

Physical Properties

Property code	Value	Unit	Source
gf	-406.79	kJ/mol	Joback Method
hf	-863.55	kJ/mol	Joback Method
hfus	40.85	kJ/mol	Joback Method
hvap	71.29	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.841		Crippen Method
mcvol	249.330	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	2006.00		NIST Webbook
tb	732.17	K	Joback Method
tc	914.96	K	Joback Method
tf	418.05	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.70	J/mol×K	732.17	Joback Method
cpg	724.18	J/mol×K	762.64	Joback Method
cpg	738.83	J/mol×K	793.10	Joback Method
cpg	752.66	J/mol×K	823.57	Joback Method
cpg	765.68	J/mol×K	854.03	Joback Method
cpg	777.89	J/mol×K	884.50	Joback Method
cpg	789.31	J/mol×K	914.96	Joback Method
dvisc	0.0013342	Pa×s	418.05	Joback Method
dvisc	0.0006557	Pa×s	470.40	Joback Method

dvisc	0.0003715	Pa×s	522.76	Joback Method
dvisc	0.0002334	Pa×s	575.11	Joback Method
dvisc	0.0001585	Pa×s	627.46	Joback Method
dvisc	0.0001142	Pa×s	679.82	Joback Method
dvisc	0.0000863	Pa×s	732.17	Joback Method

Sources

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=U349031&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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