Malonic acid, 10-chlorodecyl ethyl ester

Inchi: InChI=1S/C15H27ClO4/c1-2-19-14(17)13-15(18)20-12-10-8-6-4-3-5-7-9-11-16/h2-13H2,1
InchiKey: CYTQLGHFERDHGV-UHFFFAOYSA-N
Formula: C15H27ClO4
SMILES: CCOC(=O)CC(=O)OCCCCCCCCCCCCl
Mol. weight [g/mol]: 306.82

Physical Properties

Property code	Value	Unit	Source
gf	-404.35	kJ/mol	Joback Method
hf	-858.27	kJ/mol	Joback Method
hfus	44.38	kJ/mol	Joback Method
hvap	71.68	kJ/mol	Joback Method
log10ws	-3.98		Crippen Method
logp	3.842		Crippen Method
mcvol	249.330	ml/mol	McGowan Method
pc	1475.88	kPa	Joback Method
rinpol	2135.00		NIST Webbook
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tb	732.61	K	Joback Method
tc	913.43	K	Joback Method
tf	433.05	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	708.19	J/mol×K	732.61	Joback Method
cpg	723.48	J/mol×K	762.75	Joback Method
cpg	737.98	J/mol×K	792.88	Joback Method
cpg	751.68	J/mol×K	823.02	Joback Method
cpg	764.59	J/mol×K	853.16	Joback Method
cpg	776.72	J/mol×K	883.29	Joback Method
cpg	788.08	J/mol×K	913.43	Joback Method
dvisc	0.0011207	Pa×s	433.05	Joback Method

dvisc	0.0005981	Pa×s	482.98	Joback Method
dvisc	0.0003590	Pa×s	532.90	Joback Method
dvisc	0.0002352	Pa×s	582.83	Joback Method
dvisc	0.0001647	Pa×s	632.76	Joback Method
dvisc	0.0001215	Pa×s	682.68	Joback Method
dvisc	0.0000935	Pa×s	732.61	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=U349038&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

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