Malonic acid, 8-chlorooctyl pentyl ester

Inchi: InChI=1S/C16H29ClO4/c1-2-3-9-12-20-15(18)14-16(19)21-13-10-7-5-4-6-8-11-17/h2-14H
InchiKey: GHRBRCOZQDGBSO-UHFFFAOYSA-N
Formula: C16H29ClO4
SMILES: CCCCCOC(=O)CC(=O)OCCCCCCCCCCl
Mol. weight [g/mol]: 320.85

Physical Properties

Property code	Value	Unit	Source
gf	-395.93	kJ/mol	Joback Method
hf	-878.91	kJ/mol	Joback Method
hfus	46.97	kJ/mol	Joback Method
hvap	73.91	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	4.232		Crippen Method
mcvol	263.420	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2212.00		NIST Webbook
tb	755.49	K	Joback Method
tc	937.01	K	Joback Method
tf	444.32	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.82	J/mol×K	755.49	Joback Method
cpg	780.54	J/mol×K	785.74	Joback Method
cpg	795.41	J/mol×K	816.00	Joback Method
cpg	809.43	J/mol×K	846.25	Joback Method
cpg	822.63	J/mol×K	876.50	Joback Method
cpg	835.01	J/mol×K	906.75	Joback Method
cpg	846.57	J/mol×K	937.01	Joback Method
dvisc	0.0010176	Pa×s	444.32	Joback Method
dvisc	0.0005360	Pa×s	496.18	Joback Method

dvisc	0.0003188	Pa×s	548.04	Joback Method
dvisc	0.0002074	Pa×s	599.90	Joback Method
dvisc	0.0001445	Pa×s	651.77	Joback Method
dvisc	0.0001062	Pa×s	703.63	Joback Method
dvisc	0.0000814	Pa×s	755.49	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=U349006&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