Malonic acid, 2-chloropropyl pentadecyl ester

Inchi: InChI=1S/C21H39ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-25-20(23)17-21(24)26-18
InchiKey: DQWVDNYIQVEEMR-UHFFFAOYSA-N
Formula: C21H39ClO4
SMILES: CCCCCCCCCCCCCCCOC(=O)CC(=O)OCC(C)Cl
Mol. weight [g/mol]: 390.99

Physical Properties

Property code	Value	Unit	Source
gf	-356.27	kJ/mol	Joback Method
hf	-987.39	kJ/mol	Joback Method
hfus	56.39	kJ/mol	Joback Method
hvap	84.65	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	6.181		Crippen Method
mcvol	333.870	ml/mol	McGowan Method
pc	994.51	kPa	Joback Method
rinpol	2610.00		NIST Webbook
tb	869.45	K	Joback Method
tc	1064.76	K	Joback Method
tf	485.67	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.28	J/mol×K	869.45	Joback Method
cpg	1139.64	J/mol×K	1032.21	Joback Method
cpg	1126.44	J/mol×K	999.66	Joback Method
cpg	1112.13	J/mol×K	967.10	Joback Method
cpg	1096.68	J/mol×K	934.55	Joback Method
cpg	1080.07	J/mol×K	902.00	Joback Method
cpg	1151.76	J/mol×K	1064.76	Joback Method
dvisc	0.0000359	Pa×s	869.45	Joback Method
dvisc	0.0000482	Pa×s	805.49	Joback Method

dvisc	0.0000682	Pa×s	741.52	Joback Method
dvisc	0.0001029	Pa×s	677.56	Joback Method
dvisc	0.0001692	Pa×s	613.60	Joback Method
dvisc	0.0003124	Pa×s	549.63	Joback Method
dvisc	0.0006779	Pa×s	485.67	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=U349036&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