Adipic acid, 10-chlorodecyl hexyl ester

Inchi: InChI=1S/C22H41ClO4/c1-2-3-4-14-19-26-21(24)16-11-12-17-22(25)27-20-15-10-8-6-5-7
InchiKey: QJHMRCBMXRIYCD-UHFFFAOYSA-N
Formula: C22H41ClO4
SMILES: CCCCCCOC(=O)CCCCC(=O)OCCCCCCCCCCCl
Mol. weight [g/mol]: 405.01

Physical Properties

Property code	Value	Unit	Source
gf	-345.41	kJ/mol	Joback Method
hf	-1002.75	kJ/mol	Joback Method
hfus	62.51	kJ/mol	Joback Method
hvap	87.26	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	6.573		Crippen Method
mcvol	347.960	ml/mol	McGowan Method
pc	932.35	kPa	Joback Method
rinpol	2839.00		NIST Webbook
tb	892.77	K	Joback Method
tc	1093.16	K	Joback Method
tf	511.94	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1123.47	J/mol×K	892.77	Joback Method
cpg	1141.72	J/mol×K	926.17	Joback Method
cpg	1158.72	J/mol×K	959.57	Joback Method
cpg	1174.47	J/mol×K	992.96	Joback Method
cpg	1189.02	J/mol×K	1026.36	Joback Method
cpg	1202.40	J/mol×K	1059.76	Joback Method
cpg	1214.62	J/mol×K	1093.16	Joback Method
dvisc	0.0005220	Pa×s	511.94	Joback Method
dvisc	0.0002569	Pa×s	575.41	Joback Method

dvisc	0.0001456	Pa×s	638.88	Joback Method
dvisc	0.0000914	Pa×s	702.36	Joback Method
dvisc	0.0000620	Pa×s	765.83	Joback Method
dvisc	0.0000446	Pa×s	829.30	Joback Method
dvisc	0.0000337	Pa×s	892.77	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=U353490&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