Fumaric acid, 2-chloropropyl pentadecyl ester

Inchi: InChI=1S/C22H39ClO4/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-26-21(24)16-17-22(25)27
InchiKey: MQORINRNGKZFOW-WUKNDPDISA-N
Formula: C22H39ClO4
SMILES: CCCCCCCCCCCCCCCCOC(=O)C=CC(=O)OCC(C)Cl
Mol. weight [g/mol]: 403.00

Physical Properties

Property code	Value	Unit	Source
gf	-267.63	kJ/mol	Joback Method
hf	-890.81	kJ/mol	Joback Method
hfus	59.19	kJ/mol	Joback Method
hvap	86.83	kJ/mol	Joback Method
log10ws	-6.88		Crippen Method
logp	6.348		Crippen Method
mcvol	343.660	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	2768.00		NIST Webbook
rinpol	2768.00		NIST Webbook
tb	896.49	K	Joback Method
tc	1097.65	K	Joback Method
tf	491.86	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.81	J/mol×K	896.49	Joback Method
cpg	1114.47	J/mol×K	930.02	Joback Method
cpg	1130.95	J/mol×K	963.54	Joback Method
cpg	1146.31	J/mol×K	997.07	Joback Method
cpg	1160.57	J/mol×K	1030.60	Joback Method
cpg	1173.78	J/mol×K	1064.13	Joback Method
cpg	1185.97	J/mol×K	1097.65	Joback Method
dvisc	0.0005576	Pa×s	491.86	Joback Method

dvisc	0.0002481	Pa×s	559.30	Joback Method
dvisc	0.0001314	Pa×s	626.74	Joback Method
dvisc	0.0000787	Pa×s	694.17	Joback Method
dvisc	0.0000516	Pa×s	761.61	Joback Method
dvisc	0.0000363	Pa×s	829.05	Joback Method
dvisc	0.0000269	Pa×s	896.49	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=U348572&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