Fumaric acid, 10-chlorodecyl octyl ester

Inchi: InChI=1S/C22H39ClO4/c1-2-3-4-5-11-14-19-26-21(24)16-17-22(25)27-20-15-12-9-7-6-8-
InchiKey: LCSYCOIHYYRUDF-WUKNDPDISA-N
Formula: C22H39ClO4
SMILES: CCCCCCCCOC(=O)C=CC(=O)OCCCCCCCCCCCl
Mol. weight [g/mol]: 403.00

Physical Properties

Property code	Value	Unit	Source
gf	-265.19	kJ/mol	Joback Method
hf	-885.53	kJ/mol	Joback Method
hfus	62.71	kJ/mol	Joback Method
hvap	87.22	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	6.349		Crippen Method
mcvol	343.660	ml/mol	McGowan Method
pc	962.67	kPa	Joback Method
rinpol	2903.00		NIST Webbook
tb	896.93	K	Joback Method
tc	1098.10	K	Joback Method
tf	506.86	K	Joback Method
vc	1.345	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1096.35	J/mol×K	896.93	Joback Method
cpg	1114.04	J/mol×K	930.46	Joback Method
cpg	1130.56	J/mol×K	963.99	Joback Method
cpg	1145.96	J/mol×K	997.51	Joback Method
cpg	1160.28	J/mol×K	1031.04	Joback Method
cpg	1173.55	J/mol×K	1064.57	Joback Method
cpg	1185.83	J/mol×K	1098.10	Joback Method
dvisc	0.0004850	Pa×s	506.86	Joback Method
dvisc	0.0002331	Pa×s	571.87	Joback Method

dvisc	0.0001301	Pa×s	636.88	Joback Method
dvisc	0.0000809	Pa×s	701.89	Joback Method
dvisc	0.0000546	Pa×s	766.91	Joback Method
dvisc	0.0000391	Pa×s	831.92	Joback Method
dvisc	0.0000294	Pa×s	896.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348312&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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