Fumaric acid, 2-chlorophenyl dodec-2-en-1-yl ester

Inchi: InChI=1S/C22H29ClO4/c1-2-3-4-5-6-7-8-9-10-13-18-26-21(24)16-17-22(25)27-20-15-12-
InchiKey: QDBKPRFMAIRFGE-VTRAWOOYSA-N
Formula: C22H29ClO4
SMILES: CCCCCCCCCC=CCOC(=O)C=CC(=O)Oc1ccccc1Cl
Mol. weight [g/mol]: 392.92

Physical Properties

Property code	Value	Unit	Source
gf	-82.19	kJ/mol	Joback Method
hf	-543.25	kJ/mol	Joback Method
hfus	56.56	kJ/mol	Joback Method
hvap	90.12	kJ/mol	Joback Method
log10ws	-6.90		Crippen Method
logp	6.042		Crippen Method
mcvol	315.600	ml/mol	McGowan Method
pc	1226.84	kPa	Joback Method
rinpol	2850.00		NIST Webbook
rinpol	2850.00		NIST Webbook
tb	932.75	K	Joback Method
tc	1147.92	K	Joback Method
tf	540.72	K	Joback Method
vc	1.216	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	968.20	J/mol×K	932.75	Joback Method
cpg	982.90	J/mol×K	968.61	Joback Method
cpg	996.56	J/mol×K	1004.47	Joback Method
cpg	1009.23	J/mol×K	1040.34	Joback Method
cpg	1020.99	J/mol×K	1076.20	Joback Method
cpg	1031.90	J/mol×K	1112.06	Joback Method
cpg	1042.02	J/mol×K	1147.92	Joback Method
dvisc	0.0003311	Pa×s	540.72	Joback Method

dvisc	0.0001741	Pa×s	606.06	Joback Method
dvisc	0.0001037	Pa×s	671.40	Joback Method
dvisc	0.0000678	Pa×s	736.73	Joback Method
dvisc	0.0000474	Pa×s	802.07	Joback Method
dvisc	0.0000350	Pa×s	867.41	Joback Method
dvisc	0.0000270	Pa×s	932.75	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=U405729&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