Fumaric acid, dodecyl 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C22H28Cl4O4/c1-2-3-4-5-6-7-8-9-10-11-14-29-18(27)12-13-19(28)30-22-17(24
InchiKey: WQPUSNHVQBXBHQ-OUKQBFOZSA-N
Formula: C22H28Cl4O4
SMILES: CCCCCCCCCCCCOC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 498.27

Physical Properties

Property code	Value	Unit	Source
gf	-227.09	kJ/mol	Joback Method
hf	-742.10	kJ/mol	Joback Method
hfus	67.79	kJ/mol	Joback Method
hvap	105.30	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.226		Crippen Method
mcvol	356.620	ml/mol	McGowan Method
pc	1065.87	kPa	Joback Method
rinpol	3357.00		NIST Webbook
tb	1055.82	K	Joback Method
tc	1292.64	K	Joback Method
tf	673.12	K	Joback Method
vc	1.383	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1059.59	J/mol×K	1055.82	Joback Method
cpg	1071.01	J/mol×K	1095.29	Joback Method
cpg	1081.16	J/mol×K	1134.76	Joback Method
cpg	1090.09	J/mol×K	1174.23	Joback Method
cpg	1097.85	J/mol×K	1213.70	Joback Method
cpg	1104.48	J/mol×K	1253.17	Joback Method
cpg	1110.04	J/mol×K	1292.64	Joback Method
dvisc	0.0001375	Pa×s	673.12	Joback Method
dvisc	0.0000864	Pa×s	736.90	Joback Method

dvisc	0.0000585	Pa×s	800.69	Joback Method
dvisc	0.0000420	Pa×s	864.47	Joback Method
dvisc	0.0000315	Pa×s	928.25	Joback Method
dvisc	0.0000245	Pa×s	992.04	Joback Method
dvisc	0.0000197	Pa×s	1055.82	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=U348204&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