Fumaric acid, di(2,3,4,6-tetrachlorophenyl) ester

Inchi: InChI=1S/C16H4Cl8O4/c17-5-3-7(19)15(13(23)11(5)21)27-9(25)1-2-10(26)28-16-8(20)4-

InchiKey: XXEKWCKUIYKCMN-OWOJBTEDSA-N

Formula: C16H4Cl8O4

SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl)Oc1c(Cl)cc(Cl)c(Cl)c1Cl

Mol. weight [g/mol]: 543.83

Physical Properties

Property code	Value	Unit	Source
gf	-251.44	kJ/mol	Joback Method
hf	-490.57	kJ/mol	Joback Method
hfus	61.52	kJ/mol	Joback Method
hvap	114.41	kJ/mol	Joback Method
log10ws	-9.08		Crippen Method
logp	7.981		Crippen Method
mcvol	297.280	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinpol	3542.00		NIST Webbook
tb	1114.86	K	Joback Method
tc	1383.11	K	Joback Method
tf	801.68	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	645.10	J/mol×K	1114.86	Joback Method
cpg	647.36	J/mol×K	1159.57	Joback Method
cpg	648.51	J/mol×K	1204.28	Joback Method
cpg	648.54	J/mol×K	1248.99	Joback Method
cpg	647.47	J/mol×K	1293.69	Joback Method
cpg	645.31	J/mol×K	1338.40	Joback Method
cpg	642.08	J/mol×K	1383.11	Joback Method
dvisc	0.0000992	Pa×s	801.68	Joback Method
dvisc	0.0000756	Pa×s	853.88	Joback Method

dvisc	0.0000595	Pa×s	906.07	Joback Method
dvisc	0.0000480	Pa×s	958.27	Joback Method
dvisc	0.0000397	Pa×s	1010.47	Joback Method
dvisc	0.0000334	Pa×s	1062.66	Joback Method
dvisc	0.0000285	Pa×s	1114.86	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U348205&Units=SI

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