Fumaric acid, di(2,4,6-trichlorophenyl) ester

Inchi: InChI=1S/C16H6Cl6O4/c17-7-3-9(19)15(10(20)4-7)25-13(23)1-2-14(24)26-16-11(21)5-8(
InchiKey: PVAYWDBKLFNXLA-OWOJBTEDSA-N
Formula: C16H6Cl6O4
SMILES: O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 474.93

Physical Properties

Property code	Value	Unit	Source
gf	-208.32	kJ/mol	Joback Method
hf	-436.15	kJ/mol	Joback Method
hfus	53.90	kJ/mol	Joback Method
hvap	104.31	kJ/mol	Joback Method
log10ws	-7.71		Crippen Method
logp	6.674		Crippen Method
mcvol	272.800	ml/mol	McGowan Method
pc	1957.87	kPa	Joback Method
rinpol	3081.00		NIST Webbook
tb	1030.04	K	Joback Method
tc	1290.67	K	Joback Method
tf	716.80	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	627.63	J/mol×K	1030.04	Joback Method
cpg	632.60	J/mol×K	1073.48	Joback Method
cpg	636.51	J/mol×K	1116.92	Joback Method
cpg	639.40	J/mol×K	1160.36	Joback Method
cpg	641.30	J/mol×K	1203.79	Joback Method
cpg	642.23	J/mol×K	1247.23	Joback Method
cpg	642.22	J/mol×K	1290.67	Joback Method
dvisc	0.0001564	Pa×s	716.80	Joback Method
dvisc	0.0001142	Pa×s	769.01	Joback Method

dvisc	0.0000868	Pa×s	821.21	Joback Method
dvisc	0.0000682	Pa×s	873.42	Joback Method
dvisc	0.0000550	Pa×s	925.63	Joback Method
dvisc	0.0000455	Pa×s	977.83	Joback Method
dvisc	0.0000383	Pa×s	1030.04	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=U348280&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