Fumaric acid, 2-methylphenyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C17H11Cl3O4/c1-10-4-2-3-5-14(10)23-15(21)6-7-16(22)24-17-12(19)8-11(18)9

InchiKey: BNXQODRHCKXXSC-VOTSOKGWSA-N

Formula: C17H11Cl3O4

SMILES: Cc1ccccc1OC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 385.63

Physical Properties

Property code	Value	Unit	Source
gf	-144.85	kJ/mol	Joback Method
hf	-386.63	kJ/mol	Joback Method
hfus	44.68	kJ/mol	Joback Method
hvap	92.06	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.022		Crippen Method
mcvol	250.170	ml/mol	McGowan Method
pc	2038.23	kPa	Joback Method
rinpol	2639.00		NIST Webbook
rinpol	2639.00		NIST Webbook
tb	930.67	K	Joback Method
tc	1179.43	K	Joback Method
tf	613.27	K	Joback Method
vc	0.947	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.93	J/mol×K	930.67	Joback Method
cpg	650.97	J/mol×K	972.13	Joback Method
cpg	658.91	J/mol×K	1013.59	Joback Method
cpg	665.79	J/mol×K	1055.05	Joback Method
cpg	671.64	J/mol×K	1096.51	Joback Method
cpg	676.50	J/mol×K	1137.97	Joback Method
cpg	680.42	J/mol×K	1179.43	Joback Method
dvisc	0.0002712	Pa×s	613.27	Joback Method

dvisc	0.0001839	Pa×s	666.17	Joback Method
dvisc	0.0001320	Pa×s	719.07	Joback Method
dvisc	0.0000992	Pa×s	771.97	Joback Method
dvisc	0.0000773	Pa×s	824.87	Joback Method
dvisc	0.0000621	Pa×s	877.77	Joback Method
dvisc	0.0000511	Pa×s	930.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405689&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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