Fumaric acid, 3,5-dimethylphenyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C18H13Cl3O4/c1-10-5-11(2)7-13(6-10)24-16(22)3-4-17(23)25-18-14(20)8-12(

InchiKey: ATRFQQXXYJAUSH-ONEGZZNKSA-N

Formula: C18H13Cl3O4

SMILES: Cc1cc(C)cc(OC(=O)C=CC(=O)Oc2c(Cl)cc(Cl)cc2Cl)c1

Mol. weight [g/mol]: 399.65

Physical Properties

Property code	Value	Unit	Source
gf	-146.06	kJ/mol	Joback Method
hf	-418.74	kJ/mol	Joback Method
hfus	46.88	kJ/mol	Joback Method
hvap	94.95	kJ/mol	Joback Method
log10ws	-6.61		Crippen Method
logp	5.331		Crippen Method
mcvol	264.260	ml/mol	McGowan Method
pc	1848.33	kPa	Joback Method
rinpol	2794.00		NIST Webbook
rinpol	2794.00		NIST Webbook
tb	958.53	K	Joback Method
tc	1205.09	K	Joback Method
tf	637.06	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.73	J/mol×K	958.53	Joback Method
cpg	730.43	J/mol×K	1163.99	Joback Method
cpg	725.65	J/mol×K	1122.90	Joback Method
cpg	719.83	J/mol×K	1081.81	Joback Method
cpg	712.92	J/mol×K	1040.72	Joback Method
cpg	704.90	J/mol×K	999.62	Joback Method
cpg	734.18	J/mol×K	1205.09	Joback Method
dvisc	0.0000454	Pa×s	958.53	Joback Method

dvisc	0.0000548	Pa×s	904.95	Joback Method
dvisc	0.0000678	Pa×s	851.37	Joback Method
dvisc	0.0000861	Pa×s	797.80	Joback Method
dvisc	0.0001133	Pa×s	744.22	Joback Method
dvisc	0.0001557	Pa×s	690.64	Joback Method
dvisc	0.0002255	Pa×s	637.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405745&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

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