Fumaric acid, 2,4,6-trichlorophenyl 4-chloro-3-methylphenyl ester

Inchi: InChI=1S/C17H10Cl4O4/c1-9-6-11(2-3-12(9)19)24-15(22)4-5-16(23)25-17-13(20)7-10(18)8-14(17)21

InchiKey: OCWKLDKQHHBYFU-SNAWJCMRSA-N

Formula: C17H10Cl4O4

SMILES: Cc1cc(OC(=O)C=CC(=O)Oc2c(Cl)cc(Cl)cc2Cl)ccc1Cl

Mol. weight [g/mol]: 420.07

Physical Properties

Property code	Value	Unit	Source
gf	-166.41	kJ/mol	Joback Method
hf	-413.84	kJ/mol	Joback Method
hfus	48.49	kJ/mol	Joback Method
hvap	97.11	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.676		Crippen Method
mcvol	262.410	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	2914.00		NIST Webbook
rinpol	2914.00		NIST Webbook
tb	973.08	K	Joback Method
tc	1225.02	K	Joback Method
tf	655.71	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	656.59	J/mol×K	973.08	Joback Method
cpg	684.51	J/mol×K	1183.03	Joback Method
cpg	680.99	J/mol×K	1141.04	Joback Method
cpg	676.47	J/mol×K	1099.05	Joback Method
cpg	670.91	J/mol×K	1057.06	Joback Method
cpg	664.30	J/mol×K	1015.07	Joback Method
cpg	687.06	J/mol×K	1225.02	Joback Method
dvisc	0.0000448	Pa×s	973.08	Joback Method

dvisc	0.0000539	Pa×s	920.19	Joback Method
dvisc	0.0000663	Pa×s	867.29	Joback Method
dvisc	0.0000837	Pa×s	814.39	Joback Method
dvisc	0.0001093	Pa×s	761.50	Joback Method
dvisc	0.0001484	Pa×s	708.61	Joback Method
dvisc	0.0002116	Pa×s	655.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405959&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