Fumaric acid, 2-methylphenyl 2,3-dichlorophenyl ester

Inchi: InChI=1S/C17H12Cl2O4/c1-11-5-2-3-7-13(11)22-15(20)9-10-16(21)23-14-8-4-6-12(18)17

InchiKey: LRIFYFUTAMVXTD-MDZDMXLPSA-N

Formula: C17H12Cl2O4

SMILES: Cc1ccccc1OC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 351.18

Physical Properties

Property code	Value	Unit	Source
gf	-123.29	kJ/mol	Joback Method
hf	-359.42	kJ/mol	Joback Method
hfus	40.87	kJ/mol	Joback Method
hvap	87.01	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.369		Crippen Method
mcvol	237.930	ml/mol	McGowan Method
pc	2137.41	kPa	Joback Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook
tb	888.26	K	Joback Method
tc	1134.03	K	Joback Method
tf	570.83	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	625.47	J/mol×K	888.26	Joback Method
cpg	666.65	J/mol×K	1093.06	Joback Method
cpg	660.48	J/mol×K	1052.10	Joback Method
cpg	653.32	J/mol×K	1011.14	Joback Method
cpg	645.13	J/mol×K	970.18	Joback Method
cpg	635.86	J/mol×K	929.22	Joback Method
cpg	671.86	J/mol×K	1134.03	Joback Method
dvisc	0.0000580	Pa×s	888.26	Joback Method

dvisc	0.0000712	Pa×s	835.36	Joback Method
dvisc	0.0000898	Pa×s	782.45	Joback Method
dvisc	0.0001173	Pa×s	729.55	Joback Method
dvisc	0.0001598	Pa×s	676.64	Joback Method
dvisc	0.0002292	Pa×s	623.74	Joback Method
dvisc	0.0003516	Pa×s	570.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405687&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