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

Inchi: InChI=1S/C17H11Cl3O5/c1-23-13-4-2-3-5-14(13)24-15(21)6-7-16(22)25-17-11(19)8-10(1

InchiKey: ROICHDDDCPNCMP-VOTSOKGWSA-N

Formula: C17H11Cl3O5

SMILES: COc1ccccc1OC(=O)C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 401.62

Physical Properties

Property code	Value	Unit	Source
gf	-249.85	kJ/mol	Joback Method
hf	-518.85	kJ/mol	Joback Method
hfus	45.87	kJ/mol	Joback Method
hvap	94.47	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.723		Crippen Method
mcvol	256.040	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	2787.00		NIST Webbook
rinpol	2787.00		NIST Webbook
tb	953.09	K	Joback Method
tc	1199.77	K	Joback Method
tf	635.50	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.61	J/mol×K	953.09	Joback Method
cpg	694.62	J/mol×K	1158.65	Joback Method
cpg	691.24	J/mol×K	1117.54	Joback Method
cpg	686.67	J/mol×K	1076.43	Joback Method
cpg	680.88	J/mol×K	1035.32	Joback Method
cpg	673.87	J/mol×K	994.20	Joback Method
cpg	696.81	J/mol×K	1199.77	Joback Method
dvisc	0.0000381	Pa×s	953.09	Joback Method

dvisc	0.0000463	Pa×s	900.16	Joback Method
dvisc	0.0000574	Pa×s	847.23	Joback Method
dvisc	0.0000734	Pa×s	794.29	Joback Method
dvisc	0.0000972	Pa×s	741.36	Joback Method
dvisc	0.0001344	Pa×s	688.43	Joback Method
dvisc	0.0001961	Pa×s	635.50	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=U405940&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