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

Inchi: InChI=1S/C17H12Cl2O5/c1-22-12-6-2-3-7-13(12)23-15(20)9-10-16(21)24-14-8-4-5-11(18

InchiKey: SQRPMTQHOWJLQM-MDZDMXLPSA-N

Formula: C17H12Cl2O5

SMILES: COc1ccccc1OC(=O)C=CC(=O)Oc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 367.18

Physical Properties

Property code	Value	Unit	Source
gf	-228.29	kJ/mol	Joback Method
hf	-491.64	kJ/mol	Joback Method
hfus	42.06	kJ/mol	Joback Method
hvap	89.42	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.069		Crippen Method
mcvol	243.800	ml/mol	McGowan Method
pc	2104.20	kPa	Joback Method
rinpol	2743.00		NIST Webbook
rinpol	2743.00		NIST Webbook
tb	910.68	K	Joback Method
tc	1154.00	K	Joback Method
tf	593.06	K	Joback Method
vc	0.915	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.91	J/mol×K	910.68	Joback Method
cpg	686.46	J/mol×K	1113.45	Joback Method
cpg	681.52	J/mol×K	1072.89	Joback Method
cpg	675.42	J/mol×K	1032.34	Joback Method
cpg	668.13	J/mol×K	991.79	Joback Method
cpg	659.63	J/mol×K	951.23	Joback Method
cpg	690.25	J/mol×K	1154.00	Joback Method
dvisc	0.0000435	Pa×s	910.68	Joback Method

dvisc	0.0000533	Pa×s	857.74	Joback Method
dvisc	0.0000671	Pa×s	804.81	Joback Method
dvisc	0.0000872	Pa×s	751.87	Joback Method
dvisc	0.0001181	Pa×s	698.93	Joback Method
dvisc	0.0001678	Pa×s	646.00	Joback Method
dvisc	0.0002541	Pa×s	593.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405938&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