Fumaric acid, 2,6-dimethoxyphenyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C18H14ClFO6/c1-23-13-7-4-8-14(24-2)18(13)26-16(22)10-9-15(21)25-17-11(1

InchiKey: WTDGITNHEMVTJE-MDZDMXLPSA-N

Formula: C18H14ClFO6

SMILES: COc1cccc(OC)c1OC(=O)C=CC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 380.75

Physical Properties

Property code	Value	Unit	Source
gf	-517.38	kJ/mol	Joback Method
hf	-836.34	kJ/mol	Joback Method
hfus	44.33	kJ/mol	Joback Method
hvap	89.52	kJ/mol	Joback Method
log10ws	-4.86		Crippen Method
logp	3.563		Crippen Method
mcvol	253.290	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	2675.00		NIST Webbook
tb	922.80	K	Joback Method
tc	1153.15	K	Joback Method
tf	609.75	K	Joback Method
vc	0.959	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	716.85	J/mol×K	922.80	Joback Method
cpg	726.82	J/mol×K	961.19	Joback Method
cpg	735.46	J/mol×K	999.58	Joback Method
cpg	742.78	J/mol×K	1037.98	Joback Method
cpg	748.76	J/mol×K	1076.37	Joback Method
cpg	753.39	J/mol×K	1114.76	Joback Method
cpg	756.67	J/mol×K	1153.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405758&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
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