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

Inchi: InChI=1S/C18H15FO6/c1-22-14-8-5-9-15(23-2)18(14)25-17(21)11-10-16(20)24-13-7-4-3

InchiKey: GPRRCJQCBVYZMB-ZHACJKMWSA-N

Formula: C18H15FO6

SMILES: COc1cccc(OC)c1OC(=O)C=CC(=O)Oc1ccccc1F

Mol. weight [g/mol]: 346.31

Physical Properties

Property code	Value	Unit	Source
gf	-495.82	kJ/mol	Joback Method
hf	-809.13	kJ/mol	Joback Method
hfus	40.52	kJ/mol	Joback Method
hvap	84.47	kJ/mol	Joback Method
log10ws	-4.17		Crippen Method
logp	2.910		Crippen Method
mcvol	241.050	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	2546.00		NIST Webbook
rinpol	2546.00		NIST Webbook
tb	880.39	K	Joback Method
tc	1106.44	K	Joback Method
tf	567.31	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.21	J/mol×K	880.39	Joback Method
cpg	709.71	J/mol×K	918.07	Joback Method
cpg	719.94	J/mol×K	955.74	Joback Method
cpg	728.89	J/mol×K	993.42	Joback Method
cpg	736.56	J/mol×K	1031.09	Joback Method
cpg	742.95	J/mol×K	1068.77	Joback Method
cpg	748.06	J/mol×K	1106.44	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405755&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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