Fumaric acid, monoamide, N-(2,4-dimethoxyphenyl)-, 3-fluorophenyl ester

Inchi: InChI=1S/C18H16FNO5/c1-23-13-6-7-15(16(11-13)24-2)20-17(21)8-9-18(22)25-14-5-3-4

InchiKey: CSUQBUCVBXAXHU-CMDGGOBGSA-N

Formula: C18H16FNO5

SMILES: COc1ccc(NC(=O)C=CC(=O)Oc2cccc(F)c2)c(OC)c1

Mol. weight [g/mol]: 345.32

Physical Properties

Property code	Value	Unit	Source
gf	-301.43	kJ/mol	Joback Method
hf	-623.44	kJ/mol	Joback Method
hfus	44.43	kJ/mol	Joback Method
hvap	88.50	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	2.943		Crippen Method
mcvol	245.160	ml/mol	McGowan Method
pc	2003.70	kPa	Joback Method
rinpol	3055.00		NIST Webbook
tb	908.14	K	Joback Method
tc	1136.28	K	Joback Method
tf	597.74	K	Joback Method
vc	0.926	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	723.97	J/mol×K	908.14	Joback Method
cpg	735.08	J/mol×K	946.16	Joback Method
cpg	744.96	J/mol×K	984.19	Joback Method
cpg	753.63	J/mol×K	1022.21	Joback Method
cpg	761.12	J/mol×K	1060.23	Joback Method
cpg	767.44	J/mol×K	1098.25	Joback Method
cpg	772.62	J/mol×K	1136.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357491&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