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

Inchi: InChI=1S/C18H16ClNO5/c1-23-12-7-8-14(16(11-12)24-2)20-17(21)9-10-18(22)25-15-6-4

InchiKey: GEQGBHBVYYOJDH-MDZDMXLPSA-N

Formula: C18H16ClNO5

SMILES: COc1ccc(NC(=O)C=CC(=O)Oc2ccccc2Cl)c(OC)c1

Mol. weight [g/mol]: 361.78

Physical Properties

Property code	Value	Unit	Source
gf	-118.55	kJ/mol	Joback Method
hf	-443.07	kJ/mol	Joback Method
hfus	45.55	kJ/mol	Joback Method
hvap	93.70	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.457		Crippen Method
mcvol	255.630	ml/mol	McGowan Method
pc	2018.13	kPa	Joback Method
rinpol	3259.00		NIST Webbook
tb	946.30	K	Joback Method
tc	1184.26	K	Joback Method
tf	627.07	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.48	J/mol×K	946.30	Joback Method
cpg	746.63	J/mol×K	985.96	Joback Method
cpg	755.48	J/mol×K	1025.62	Joback Method
cpg	763.07	J/mol×K	1065.28	Joback Method
cpg	769.41	J/mol×K	1104.94	Joback Method
cpg	774.53	J/mol×K	1144.60	Joback Method
cpg	778.46	J/mol×K	1184.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357429&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