Fumaric acid, monoamide, N-(5-chloro-2-methoxyphenyl)-, 2-fluorophenyl ester

Inchi: InChI=1S/C17H13ClFNO4/c1-23-15-7-6-11(18)10-13(15)20-16(21)8-9-17(22)24-14-5-3-2
InchiKey: JORCQXPVUNPIJB-CMDGGOBGSA-N
Formula: C17H13ClFNO4
SMILES: COc1ccc(Cl)cc1NC(=O)C=CC(=O)Oc1ccccc1F
Mol. weight [g/mol]: 349.74

Physical Properties

Property code	Value	Unit	Source
gf	-216.78	kJ/mol	Joback Method
hf	-486.32	kJ/mol	Joback Method
hfus	44.85	kJ/mol	Joback Method
hvap	88.25	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.588		Crippen Method
mcvol	237.440	ml/mol	McGowan Method
pc	2147.32	kPa	Joback Method
rinpol	3054.00		NIST Webbook
rinpol	3054.00		NIST Webbook
tb	900.27	K	Joback Method
tc	1134.70	K	Joback Method
tf	594.16	K	Joback Method
vc	0.901	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	662.76	J/mol×K	900.27	Joback Method
cpg	673.05	J/mol×K	939.34	Joback Method
cpg	682.26	J/mol×K	978.41	Joback Method
cpg	690.42	J/mol×K	1017.49	Joback Method
cpg	697.57	J/mol×K	1056.56	Joback Method
cpg	703.76	J/mol×K	1095.63	Joback Method
cpg	709.02	J/mol×K	1134.70	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357482&Units=SI

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