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

Inchi: InChI=1S/C16H11F2NO3/c17-11-4-3-5-12(10-11)22-16(21)9-8-15(20)19-14-7-2-1-6-13(1

InchiKey: RHYJMCYJRHGUMG-CMDGGOBGSA-N

Formula: C16H11F2NO3

SMILES: O=C(C=CC(=O)Oc1cccc(F)c1)Nc1ccccc1F

Mol. weight [g/mol]: 303.26

Physical Properties

Property code	Value	Unit	Source
gf	-293.45	kJ/mol	Joback Method
hf	-502.36	kJ/mol	Joback Method
hfus	40.35	kJ/mol	Joback Method
hvap	77.75	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	3.065		Crippen Method
mcvol	207.010	ml/mol	McGowan Method
pc	2407.64	kPa	Joback Method
rinpol	2479.00		NIST Webbook
rinpol	2479.00		NIST Webbook
tb	811.83	K	Joback Method
tc	1039.56	K	Joback Method
tf	518.81	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.68	J/mol×K	811.83	Joback Method
cpg	582.99	J/mol×K	849.79	Joback Method
cpg	593.31	J/mol×K	887.74	Joback Method
cpg	602.71	J/mol×K	925.70	Joback Method
cpg	611.23	J/mol×K	963.65	Joback Method
cpg	618.95	J/mol×K	1001.61	Joback Method
cpg	625.92	J/mol×K	1039.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357486&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