Fumaric acid, monoamide, N-methyl-N-phenyl-, 3-fluorophenyl ester

Inchi: InChI=1S/C17H14FNO3/c1-19(14-7-3-2-4-8-14)16(20)10-11-17(21)22-15-9-5-6-13(18)12

InchiKey: SPPVKBQXSCUFGH-ZHACJKMWSA-N

Formula: C17H14FNO3

SMILES: CN(C(=O)C=CC(=O)Oc1cccc(F)c1)c1ccccc1

Mol. weight [g/mol]: 299.30

Physical Properties

Property code	Value	Unit	Source
gf	-59.20	kJ/mol	Joback Method
hf	-301.36	kJ/mol	Joback Method
hfus	38.17	kJ/mol	Joback Method
hvap	75.74	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.950		Crippen Method
mcvol	219.330	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	2432.00		NIST Webbook
rinpol	2432.00		NIST Webbook
tb	792.73	K	Joback Method
tc	1023.22	K	Joback Method
tf	496.78	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	608.49	J/mol×K	792.73	Joback Method
cpg	621.63	J/mol×K	831.15	Joback Method
cpg	633.67	J/mol×K	869.56	Joback Method
cpg	644.68	J/mol×K	907.98	Joback Method
cpg	654.74	J/mol×K	946.39	Joback Method
cpg	663.93	J/mol×K	984.81	Joback Method
cpg	672.33	J/mol×K	1023.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357485&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