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

Inchi: InChI=1S/C16H11ClFNO3/c17-11-4-6-13(7-5-11)19-15(20)8-9-16(21)22-14-3-1-2-12(18)10-14/h1-10,19H/b9-8-

InchiKey: LQWOZUXEHMZBQU-CMDGGOBGSA-N

Formula: C16H11ClFNO3

SMILES: O=C(C=CC(=O)Oc1cccc(F)c1)Nc1ccc(Cl)cc1

Mol. weight [g/mol]: 319.71

Physical Properties

Property code	Value	Unit	Source
gf	-110.57	kJ/mol	Joback Method
hf	-321.99	kJ/mol	Joback Method
hfus	41.46	kJ/mol	Joback Method
hvap	82.95	kJ/mol	Joback Method
log10ws	-4.51		Crippen Method
logp	3.579		Crippen Method
mcvol	217.480	ml/mol	McGowan Method
pc	2426.65	kPa	Joback Method
rinpol	2897.00		NIST Webbook
tb	849.99	K	Joback Method
tc	1088.74	K	Joback Method
tf	548.14	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	584.79	J/mol×K	849.99	Joback Method
cpg	595.42	J/mol×K	889.78	Joback Method
cpg	605.04	J/mol×K	929.57	Joback Method
cpg	613.74	J/mol×K	969.37	Joback Method
cpg	621.57	J/mol×K	1009.16	Joback Method
cpg	628.61	J/mol×K	1048.95	Joback Method
cpg	634.92	J/mol×K	1088.74	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=U357489&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