Fumaric acid, monoamide, N-(2-fluorophenyl)-, 4-chloro-3-methylphenyl ester

Inchi: InChI=1S/C17H13ClFNO3/c1-11-10-12(6-7-13(11)18)23-17(22)9-8-16(21)20-15-5-3-2-4-

InchiKey: NMBCZTDHGNNYTG-CMDGGOBGSA-N

Formula: C17H13ClFNO3

SMILES: Cc1cc(OC(=O)C=CC(=O)Nc2ccccc2F)ccc1Cl

Mol. weight [g/mol]: 333.74

Physical Properties

Property code	Value	Unit	Source
gf	-111.78	kJ/mol	Joback Method
hf	-354.10	kJ/mol	Joback Method
hfus	43.66	kJ/mol	Joback Method
hvap	85.84	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.888		Crippen Method
mcvol	231.570	ml/mol	McGowan Method
pc	2181.56	kPa	Joback Method
rinpol	2882.00		NIST Webbook
rinpol	2882.00		NIST Webbook
tb	877.85	K	Joback Method
tc	1114.06	K	Joback Method
tf	571.93	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.86	J/mol×K	877.85	Joback Method
cpg	648.73	J/mol×K	917.22	Joback Method
cpg	658.60	J/mol×K	956.59	Joback Method
cpg	667.52	J/mol×K	995.95	Joback Method
cpg	675.57	J/mol×K	1035.32	Joback Method
cpg	682.80	J/mol×K	1074.69	Joback Method
cpg	689.27	J/mol×K	1114.06	Joback Method

Sources

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=U357442&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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