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

Inchi: InChI=1S/C18H16FNO3/c1-2-13-6-3-4-9-16(13)20-17(21)10-11-18(22)23-15-8-5-7-14(19

InchiKey: OLJHXUNYDJBYJE-ZHACJKMWSA-N

Formula: C18H16FNO3

SMILES: CCc1ccccc1NC(=O)C=CC(=O)Oc1cccc(F)c1

Mol. weight [g/mol]: 313.32

Physical Properties

Property code	Value	Unit	Source
gf	-81.80	kJ/mol	Joback Method
hf	-347.53	kJ/mol	Joback Method
hfus	42.45	kJ/mol	Joback Method
hvap	83.02	kJ/mol	Joback Method
log10ws	-4.63		Crippen Method
logp	3.488		Crippen Method
mcvol	233.420	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	2693.00		NIST Webbook
tb	858.32	K	Joback Method
tc	1088.20	K	Joback Method
tf	540.76	K	Joback Method
vc	0.890	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.89	J/mol×K	858.32	Joback Method
cpg	686.32	J/mol×K	896.63	Joback Method
cpg	697.68	J/mol×K	934.95	Joback Method
cpg	708.06	J/mol×K	973.26	Joback Method
cpg	717.51	J/mol×K	1011.58	Joback Method
cpg	726.10	J/mol×K	1049.89	Joback Method
cpg	733.90	J/mol×K	1088.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357487&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

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