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

Inchi: InChI=1S/C13H14FNO3/c1-9(2)18-13(17)8-7-12(16)15-11-6-4-3-5-10(11)14/h3-9H,1-2H
InchiKey: OFWWGYQJWWNCEP-BQYQJAHWSA-N
Formula: C13H14FNO3
SMILES: CC(C)OC(=O)C=CC(=O)Nc1ccccc1F
Mol. weight [g/mol]: 251.25

Physical Properties

Property code	Value	Unit	Source
gf	-229.12	kJ/mol	Joback Method
hf	-474.67	kJ/mol	Joback Method
hfus	32.32	kJ/mol	Joback Method
hvap	68.56	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.272		Crippen Method
mcvol	186.730	ml/mol	McGowan Method
pc	2467.81	kPa	Joback Method
rinpol	1982.00		NIST Webbook
rinpol	1982.00		NIST Webbook
tb	711.82	K	Joback Method
tc	924.94	K	Joback Method
tf	430.47	K	Joback Method
vc	0.713	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.72	J/mol×K	711.82	Joback Method
cpg	511.48	J/mol×K	747.34	Joback Method
cpg	523.36	J/mol×K	782.86	Joback Method
cpg	534.40	J/mol×K	818.38	Joback Method
cpg	544.62	J/mol×K	853.90	Joback Method
cpg	554.06	J/mol×K	889.42	Joback Method
cpg	562.77	J/mol×K	924.94	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357522&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