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

Inchi: InChI=1S/C15H18FNO3/c1-3-6-11(2)20-15(19)10-9-14(18)17-13-8-5-4-7-12(13)16/h4-5,
InchiKey: ADIFTWWNOSFOJS-MDZDMXLPSA-N
Formula: C15H18FNO3
SMILES: CCCC(C)OC(=O)C=CC(=O)Nc1ccccc1F
Mol. weight [g/mol]: 279.31

Physical Properties

Property code	Value	Unit	Source
gf	-212.28	kJ/mol	Joback Method
hf	-515.95	kJ/mol	Joback Method
hfus	37.50	kJ/mol	Joback Method
hvap	73.01	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	3.052		Crippen Method
mcvol	214.910	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	2182.00		NIST Webbook
tb	757.58	K	Joback Method
tc	965.58	K	Joback Method
tf	453.01	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	605.02	J/mol×K	757.58	Joback Method
cpg	618.61	J/mol×K	792.25	Joback Method
cpg	631.28	J/mol×K	826.91	Joback Method
cpg	643.06	J/mol×K	861.58	Joback Method
cpg	654.00	J/mol×K	896.25	Joback Method
cpg	664.13	J/mol×K	930.91	Joback Method
cpg	673.50	J/mol×K	965.58	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=U357494&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