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

Inchi: InChI=1S/C18H24FNO3/c1-3-5-8-14(4-2)13-23-18(22)12-11-17(21)20-16-10-7-6-9-15(16

InchiKey: ZIEAWDRMBBMLPE-VAWYXSNFSA-N

Formula: C18H24FNO3

SMILES: CCCCC(CC)COC(=O)C=CC(=O)Nc1ccccc1F

Mol. weight [g/mol]: 321.39

Physical Properties

Property code	Value	Unit	Source
gf	-187.02	kJ/mol	Joback Method
hf	-577.87	kJ/mol	Joback Method
hfus	45.27	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	4.080		Crippen Method
mcvol	257.180	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	2518.00		NIST Webbook
tb	826.22	K	Joback Method
tc	1030.55	K	Joback Method
tf	486.82	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	772.51	J/mol×K	826.22	Joback Method
cpg	787.04	J/mol×K	860.28	Joback Method
cpg	800.58	J/mol×K	894.33	Joback Method
cpg	813.19	J/mol×K	928.39	Joback Method
cpg	824.91	J/mol×K	962.44	Joback Method
cpg	835.78	J/mol×K	996.50	Joback Method
cpg	845.86	J/mol×K	1030.55	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=U357506&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