Fumaric acid, 2,4,4-trimethylpentyl 2-fluorophenyl ester

Inchi: InChI=1S/C18H23FO4/c1-13(11-18(2,3)4)12-22-16(20)9-10-17(21)23-15-8-6-5-7-14(15)1

InchiKey: PLUYXWWNOGFGMW-MDZDMXLPSA-N

Formula: C18H23FO4

SMILES: CC(COC(=O)C=CC(=O)Oc1ccccc1F)CC(C)(C)C

Mol. weight [g/mol]: 322.37

Physical Properties

Property code	Value	Unit	Source
gf	-378.57	kJ/mol	Joback Method
hf	-772.31	kJ/mol	Joback Method
hfus	33.95	kJ/mol	Joback Method
hvap	74.37	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.903		Crippen Method
mcvol	253.070	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2111.00		NIST Webbook
rinpol	2111.00		NIST Webbook
tb	795.24	K	Joback Method
tc	1004.01	K	Joback Method
tf	458.81	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.46	J/mol×K	795.24	Joback Method
cpg	760.54	J/mol×K	830.04	Joback Method
cpg	774.56	J/mol×K	864.83	Joback Method
cpg	787.57	J/mol×K	899.63	Joback Method
cpg	799.63	J/mol×K	934.42	Joback Method
cpg	810.78	J/mol×K	969.22	Joback Method
cpg	821.08	J/mol×K	1004.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405607&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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