Fumaric acid, 2-ethylhexyl 2-fluorophenyl ester

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

InchiKey: DMBSLJMMWFRZAK-VAWYXSNFSA-N

Formula: C18H23FO4

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

Mol. weight [g/mol]: 322.37

Physical Properties

Property code	Value	Unit	Source
gf	-381.41	kJ/mol	Joback Method
hf	-763.56	kJ/mol	Joback Method
hfus	41.36	kJ/mol	Joback Method
hvap	75.67	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.047		Crippen Method
mcvol	253.070	ml/mol	McGowan Method
pc	1570.96	kPa	Joback Method
rinpol	2176.00		NIST Webbook
rinpol	2176.00		NIST Webbook
tb	798.47	K	Joback Method
tc	1000.03	K	Joback Method
tf	456.39	K	Joback Method
vc	0.976	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.83	J/mol×K	798.47	Joback Method
cpg	758.67	J/mol×K	832.06	Joback Method
cpg	772.52	J/mol×K	865.66	Joback Method
cpg	785.39	J/mol×K	899.25	Joback Method
cpg	797.32	J/mol×K	932.84	Joback Method
cpg	808.34	J/mol×K	966.44	Joback Method
cpg	818.47	J/mol×K	1000.03	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405574&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