Fumaric acid, 2-methylpentyl 2-fluorophenyl ester

Inchi: InChI=1S/C16H19FO4/c1-3-6-12(2)11-20-15(18)9-10-16(19)21-14-8-5-4-7-13(14)17/h4-5

InchiKey: QGXPLQUPUVBVQO-MDZDMXLPSA-N

Formula: C16H19FO4

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

Mol. weight [g/mol]: 294.32

Physical Properties

Property code	Value	Unit	Source
gf	-398.25	kJ/mol	Joback Method
hf	-722.28	kJ/mol	Joback Method
hfus	36.18	kJ/mol	Joback Method
hvap	71.21	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.267		Crippen Method
mcvol	224.890	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2003.00		NIST Webbook
rinpol	2003.00		NIST Webbook
tb	752.71	K	Joback Method
tc	956.70	K	Joback Method
tf	433.85	K	Joback Method
vc	0.864	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	632.25	J/mol×K	752.71	Joback Method
cpg	646.49	J/mol×K	786.71	Joback Method
cpg	659.78	J/mol×K	820.71	Joback Method
cpg	672.16	J/mol×K	854.71	Joback Method
cpg	683.64	J/mol×K	888.71	Joback Method
cpg	694.25	J/mol×K	922.71	Joback Method
cpg	704.02	J/mol×K	956.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405647&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