Fumaric acid, 4-methoxyphenyl 2-fluorophenyl ester

Inchi: InChI=1S/C17H13FO5/c1-21-12-6-8-13(9-7-12)22-16(19)10-11-17(20)23-15-5-3-2-4-14(1

InchiKey: GDDLKFXMRSJHNI-ZHACJKMWSA-N

Formula: C17H13FO5

SMILES: COc1ccc(OC(=O)C=CC(=O)Oc2ccccc2F)cc1

Mol. weight [g/mol]: 316.28

Physical Properties

Property code	Value	Unit	Source
gf	-389.61	kJ/mol	Joback Method
hf	-644.80	kJ/mol	Joback Method
hfus	37.13	kJ/mol	Joback Method
hvap	79.17	kJ/mol	Joback Method
log10ws	-4.05		Crippen Method
logp	2.901		Crippen Method
mcvol	221.090	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	2416.00		NIST Webbook
rinpol	2416.00		NIST Webbook
tb	830.11	K	Joback Method
tc	1059.39	K	Joback Method
tf	521.29	K	Joback Method
vc	0.836	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	618.55	J/mol×K	830.11	Joback Method
cpg	630.57	J/mol×K	868.32	Joback Method
cpg	641.43	J/mol×K	906.54	Joback Method
cpg	651.16	J/mol×K	944.75	Joback Method
cpg	659.78	J/mol×K	982.96	Joback Method
cpg	667.31	J/mol×K	1021.18	Joback Method
cpg	673.76	J/mol×K	1059.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405781&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

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