Fumaric acid, 1-phenylprop-1-yl 2-fluorophenyl ester

Inchi: InChI=1S/C19H17FO4/c1-2-16(14-8-4-3-5-9-14)23-18(21)12-13-19(22)24-17-11-7-6-10-1

InchiKey: SMRYFGPFDCSYMG-OUKQBFOZSA-N

Formula: C19H17FO4

SMILES: CCC(OC(=O)C=CC(=O)Oc1ccccc1F)c1ccccc1

Mol. weight [g/mol]: 328.33

Physical Properties

Property code	Value	Unit	Source
gf	-260.58	kJ/mol	Joback Method
hf	-547.67	kJ/mol	Joback Method
hfus	37.99	kJ/mol	Joback Method
hvap	80.17	kJ/mol	Joback Method
log10ws	-5.00		Crippen Method
logp	3.982		Crippen Method
mcvol	243.400	ml/mol	McGowan Method
pc	1910.24	kPa	Joback Method
rinpol	2344.00		NIST Webbook
rinpol	2344.00		NIST Webbook
tb	848.03	K	Joback Method
tc	1076.26	K	Joback Method
tf	494.08	K	Joback Method
vc	0.923	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	705.45	J/mol×K	848.03	Joback Method
cpg	718.70	J/mol×K	886.07	Joback Method
cpg	730.77	J/mol×K	924.11	Joback Method
cpg	741.71	J/mol×K	962.15	Joback Method
cpg	751.58	J/mol×K	1000.18	Joback Method
cpg	760.43	J/mol×K	1038.22	Joback Method
cpg	768.32	J/mol×K	1076.26	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=U405901&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