Fumaric acid, 3-phenylpropyl 2-fluorophenyl ester

Inchi: InChI=1S/C19H17FO4/c20-16-10-4-5-11-17(16)24-19(22)13-12-18(21)23-14-6-9-15-7-2-

InchiKey: JGNFRWZJMDLAQS-OUKQBFOZSA-N

Formula: C19H17FO4

SMILES: O=C(C=CC(=O)Oc1ccccc1F)OCCCc1ccccc1

Mol. weight [g/mol]: 328.33

Physical Properties

Property code	Value	Unit	Source
gf	-258.14	kJ/mol	Joback Method
hf	-542.39	kJ/mol	Joback Method
hfus	41.52	kJ/mol	Joback Method
hvap	80.55	kJ/mol	Joback Method
log10ws	-4.54		Crippen Method
logp	3.463		Crippen Method
mcvol	243.400	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinpol	2476.00		NIST Webbook
rinpol	2476.00		NIST Webbook
tb	848.47	K	Joback Method
tc	1073.51	K	Joback Method
tf	509.08	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.88	J/mol×K	848.47	Joback Method
cpg	717.96	J/mol×K	885.98	Joback Method
cpg	729.92	J/mol×K	923.48	Joback Method
cpg	740.78	J/mol×K	960.99	Joback Method
cpg	750.62	J/mol×K	998.50	Joback Method
cpg	759.48	J/mol×K	1036.01	Joback Method
cpg	767.41	J/mol×K	1073.51	Joback Method

Sources

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=U405666&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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