Fumaric acid, 2-phenethyl 2-fluorophenyl ester

Inchi: InChI=1S/C18H15FO4/c19-15-8-4-5-9-16(15)23-18(21)11-10-17(20)22-13-12-14-6-2-1-3
InchiKey: CZALSJWRFPJZDH-ZHACJKMWSA-N
Formula: C18H15FO4
SMILES: O=C(C=CC(=O)Oc1ccccc1F)OCCc1ccccc1
Mol. weight [g/mol]: 314.31

Physical Properties

Property code	Value	Unit	Source
gf	-266.56	kJ/mol	Joback Method
hf	-521.75	kJ/mol	Joback Method
hfus	38.92	kJ/mol	Joback Method
hvap	78.33	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.073		Crippen Method
mcvol	229.310	ml/mol	McGowan Method
pc	2066.12	kPa	Joback Method
rinpol	2345.00		NIST Webbook
rinpol	2345.00		NIST Webbook
tb	825.59	K	Joback Method
tc	1053.23	K	Joback Method
tf	497.81	K	Joback Method
vc	0.874	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	649.17	J/mol×K	825.59	Joback Method
cpg	662.05	J/mol×K	863.53	Joback Method
cpg	673.80	J/mol×K	901.47	Joback Method
cpg	684.47	J/mol×K	939.41	Joback Method
cpg	694.11	J/mol×K	977.35	Joback Method
cpg	702.78	J/mol×K	1015.29	Joback Method
cpg	710.53	J/mol×K	1053.23	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=U405680&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