Fumaric acid, 2-phenethyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C18H14ClFO4/c19-14-7-4-8-15(20)18(14)24-17(22)10-9-16(21)23-12-11-13-5-

InchiKey: AQCUXUSJLIFROK-MDZDMXLPSA-N

Formula: C18H14ClFO4

SMILES: O=C(C=CC(=O)Oc1c(F)cccc1Cl)OCCc1ccccc1

Mol. weight [g/mol]: 348.75

Physical Properties

Property code	Value	Unit	Source
gf	-288.12	kJ/mol	Joback Method
hf	-548.96	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	83.38	kJ/mol	Joback Method
log10ws	-4.81		Crippen Method
logp	3.727		Crippen Method
mcvol	241.550	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2480.00		NIST Webbook
rinpol	2480.00		NIST Webbook
tb	868.00	K	Joback Method
tc	1099.27	K	Joback Method
tf	540.25	K	Joback Method
vc	0.922	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.68	J/mol×K	868.00	Joback Method
cpg	681.18	J/mol×K	906.55	Joback Method
cpg	691.60	J/mol×K	945.09	Joback Method
cpg	700.96	J/mol×K	983.64	Joback Method
cpg	709.33	J/mol×K	1022.18	Joback Method
cpg	716.74	J/mol×K	1060.73	Joback Method
cpg	723.25	J/mol×K	1099.27	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405683&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