Fumaric acid, 3-phenylpropyl 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C19H16ClFO4/c20-15-9-4-10-16(21)19(15)25-18(23)12-11-17(22)24-13-5-8-14

InchiKey: RDDTXQCMDJQJBP-VAWYXSNFSA-N

Formula: C19H16ClFO4

SMILES: O=C(C=CC(=O)Oc1c(F)cccc1Cl)OCCCc1ccccc1

Mol. weight [g/mol]: 362.78

Physical Properties

Property code	Value	Unit	Source
gf	-279.70	kJ/mol	Joback Method
hf	-569.60	kJ/mol	Joback Method
hfus	45.32	kJ/mol	Joback Method
hvap	85.60	kJ/mol	Joback Method
log10ws	-5.23		Crippen Method
logp	4.117		Crippen Method
mcvol	255.640	ml/mol	McGowan Method
pc	1813.86	kPa	Joback Method
rinpol	2611.00		NIST Webbook
rinpol	2611.00		NIST Webbook
tb	890.88	K	Joback Method
tc	1119.91	K	Joback Method
tf	551.52	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.60	J/mol×K	890.88	Joback Method
cpg	737.33	J/mol×K	929.05	Joback Method
cpg	747.95	J/mol×K	967.22	Joback Method
cpg	757.51	J/mol×K	1005.40	Joback Method
cpg	766.07	J/mol×K	1043.57	Joback Method
cpg	773.66	J/mol×K	1081.74	Joback Method
cpg	780.36	J/mol×K	1119.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405669&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