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

Inchi: InChI=1S/C15H16ClFO4/c1-3-5-10(2)20-13(18)8-9-14(19)21-15-11(16)6-4-7-12(15)17/h4

InchiKey: NAMUSLVBSPAJAQ-CMDGGOBGSA-N

Formula: C15H16ClFO4

SMILES: CCCC(C)OC(=O)C=CC(=O)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 314.74

Physical Properties

Property code	Value	Unit	Source
gf	-428.23	kJ/mol	Joback Method
hf	-728.85	kJ/mol	Joback Method
hfus	37.40	kJ/mol	Joback Method
hvap	74.03	kJ/mol	Joback Method
log10ws	-4.56		Crippen Method
logp	3.672		Crippen Method
mcvol	223.040	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	772.24	K	Joback Method
tc	982.53	K	Joback Method
tf	465.02	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	602.04	J/mol×K	772.24	Joback Method
cpg	614.73	J/mol×K	807.29	Joback Method
cpg	626.52	J/mol×K	842.34	Joback Method
cpg	637.43	J/mol×K	877.39	Joback Method
cpg	647.47	J/mol×K	912.43	Joback Method
cpg	656.67	J/mol×K	947.48	Joback Method
cpg	665.05	J/mol×K	982.53	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405561&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