3-Chloro-2-fluorobenzoic acid, 2-(1-phenyleth-1-yl)-4-methoxyphenyl ester

Inchi: InChI=1S/C22H18ClFO3/c1-14(15-7-4-3-5-8-15)18-13-16(26-2)11-12-20(18)27-22(25)17

InchiKey: FUZXJQGZLVYYLG-UHFFFAOYSA-N

Formula: C22H18ClFO3

SMILES: COc1ccc(OC(=O)c2cccc(Cl)c2F)c(C(C)c2ccccc2)c1

Mol. weight [g/mol]: 384.83

Physical Properties

Property code	Value	Unit	Source
gf	-115.03	kJ/mol	Joback Method
hf	-427.85	kJ/mol	Joback Method
hfus	41.03	kJ/mol	Joback Method
hvap	88.79	kJ/mol	Joback Method
log10ws	-7.18		Crippen Method
logp	5.859		Crippen Method
mcvol	276.880	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2877.00		NIST Webbook
tb	937.69	K	Joback Method
tc	1182.51	K	Joback Method
tf	576.94	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	810.43	J/mol×K	937.69	Joback Method
cpg	822.64	J/mol×K	978.49	Joback Method
cpg	833.40	J/mol×K	1019.30	Joback Method
cpg	842.75	J/mol×K	1060.10	Joback Method
cpg	850.75	J/mol×K	1100.90	Joback Method
cpg	857.45	J/mol×K	1141.71	Joback Method
cpg	862.89	J/mol×K	1182.51	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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