Cyclopropanecarboxylic acid, trans-2-phenyl-, 2-chloro-6-fluorophenyl ester

Inchi: InChI=1S/C16H12ClFO2/c17-13-7-4-8-14(18)15(13)20-16(19)12-9-11(12)10-5-2-1-3-6-1

InchiKey: XFFAENGOSRSITO-UHFFFAOYSA-N

Formula: C16H12ClFO2

SMILES: O=C(Oc1c(F)cccc1Cl)C1CC1c1ccccc1

Mol. weight [g/mol]: 290.72

Physical Properties

Property code	Value	Unit	Source
gf	-98.22	kJ/mol	Joback Method
hf	-327.64	kJ/mol	Joback Method
hfus	33.77	kJ/mol	Joback Method
hvap	69.41	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.188		Crippen Method
mcvol	199.370	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	2134.00		NIST Webbook
rinpol	2134.00		NIST Webbook
tb	743.86	K	Joback Method
tc	985.43	K	Joback Method
tf	464.33	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.48	J/mol×K	743.86	Joback Method
cpg	551.94	J/mol×K	784.12	Joback Method
cpg	565.19	J/mol×K	824.38	Joback Method
cpg	577.32	J/mol×K	864.65	Joback Method
cpg	588.41	J/mol×K	904.91	Joback Method
cpg	598.53	J/mol×K	945.17	Joback Method
cpg	607.77	J/mol×K	985.43	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=U406843&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