Succinic acid, 2-chloro-6-fluorophenyl 4-biphenyl ester

Inchi: InChI=1S/C22H16ClFO4/c23-18-7-4-8-19(24)22(18)28-21(26)14-13-20(25)27-17-11-9-16

InchiKey: LYMKUQOTKSJLCF-UHFFFAOYSA-N

Formula: C22H16ClFO4

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)Oc1ccc(-c2ccccc2)cc1

Mol. weight [g/mol]: 398.81

Physical Properties

Property code	Value	Unit	Source
gf	-231.88	kJ/mol	Joback Method
hf	-523.68	kJ/mol	Joback Method
hfus	46.54	kJ/mol	Joback Method
hvap	95.26	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	5.437		Crippen Method
mcvol	278.450	ml/mol	McGowan Method
pc	1777.34	kPa	Joback Method
rinpol	3250.00		NIST Webbook
rinpol	3250.00		NIST Webbook
tb	987.02	K	Joback Method
tc	1233.64	K	Joback Method
tf	629.35	K	Joback Method
vc	1.058	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	816.73	J/mol×K	987.02	Joback Method
cpg	826.63	J/mol×K	1028.12	Joback Method
cpg	835.12	J/mol×K	1069.23	Joback Method
cpg	842.28	J/mol×K	1110.33	Joback Method
cpg	848.16	J/mol×K	1151.43	Joback Method
cpg	852.81	J/mol×K	1192.54	Joback Method
cpg	856.30	J/mol×K	1233.64	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390089&Units=SI

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