Succinic acid, 2-chloro-6-fluorophenyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C23H18ClFO5/c24-19-10-5-11-20(25)23(19)30-22(27)13-12-21(26)28-15-16-6

InchiKey: YBLNWBYAPHTGPL-UHFFFAOYSA-N

Formula: C23H18ClFO5

SMILES: O=C(CCC(=O)Oc1c(F)cccc1Cl)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 428.84

Physical Properties

Property code	Value	Unit	Source
gf	-328.46	kJ/mol	Joback Method
hf	-676.54	kJ/mol	Joback Method
hfus	50.32	kJ/mol	Joback Method
hvap	99.90	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.700		Crippen Method
mcvol	298.410	ml/mol	McGowan Method
pc	1619.37	kPa	Joback Method
rinpol	3126.00		NIST Webbook
rinpol	3126.00		NIST Webbook
tb	1032.32	K	Joback Method
tc	1277.55	K	Joback Method
tf	662.85	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.10	J/mol×K	1032.32	Joback Method
cpg	906.75	J/mol×K	1073.19	Joback Method
cpg	913.81	J/mol×K	1114.06	Joback Method
cpg	919.33	J/mol×K	1154.94	Joback Method
cpg	923.33	J/mol×K	1195.81	Joback Method
cpg	925.86	J/mol×K	1236.68	Joback Method
cpg	926.96	J/mol×K	1277.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390374&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