Succinic acid, 2-chloro-6-fluorophenyl pentafluorophenyl ester

Inchi: InChI=1S/C16H7ClF6O4/c17-6-2-1-3-7(18)15(6)26-8(24)4-5-9(25)27-16-13(22)11(20)10(

InchiKey: RHPSIAFXFYJZGT-UHFFFAOYSA-N

Formula: C16H7ClF6O4

SMILES: O=C(CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)Oc1c(F)cccc1Cl

Mol. weight [g/mol]: 412.67

Physical Properties

Property code	Value	Unit	Source
gf	-1407.38	kJ/mol	Joback Method
hf	-1662.80	kJ/mol	Joback Method
hfus	50.81	kJ/mol	Joback Method
hvap	78.19	kJ/mol	Joback Method
log10ws	-6.42		Crippen Method
logp	4.466		Crippen Method
mcvol	226.520	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2059.00		NIST Webbook
rinpol	2059.00		NIST Webbook
tb	839.33	K	Joback Method
tc	1041.55	K	Joback Method
tf	588.34	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.79	J/mol×K	839.33	Joback Method
cpg	625.83	J/mol×K	873.03	Joback Method
cpg	634.02	J/mol×K	906.74	Joback Method
cpg	641.35	J/mol×K	940.44	Joback Method
cpg	647.82	J/mol×K	974.15	Joback Method
cpg	653.41	J/mol×K	1007.85	Joback Method
cpg	658.12	J/mol×K	1041.55	Joback Method

Sources

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=U390353&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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