Succinic acid, 2,4,6-trichlorophenyl pentafluorophenyl ester

Inchi: InChI=1S/C16H6Cl3F5O4/c17-5-3-6(18)15(7(19)4-5)27-8(25)1-2-9(26)28-16-13(23)11(21
InchiKey: QZQFZGZNPZIYTM-UHFFFAOYSA-N
Formula: C16H6Cl3F5O4
SMILES: O=C(CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 463.57

Physical Properties

Property code	Value	Unit	Source
gf	-1246.06	kJ/mol	Joback Method
hf	-1509.64	kJ/mol	Joback Method
hfus	55.73	kJ/mol	Joback Method
hvap	88.44	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	5.634		Crippen Method
mcvol	249.230	ml/mol	McGowan Method
pc	1657.84	kPa	Joback Method
rinpol	2347.00		NIST Webbook
tb	919.90	K	Joback Method
tc	1137.17	K	Joback Method
tf	660.11	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.25	J/mol×K	919.90	Joback Method
cpg	651.34	J/mol×K	956.11	Joback Method
cpg	657.45	J/mol×K	992.32	Joback Method
cpg	662.55	J/mol×K	1028.53	Joback Method
cpg	666.65	J/mol×K	1064.75	Joback Method
cpg	669.72	J/mol×K	1100.96	Joback Method
cpg	671.76	J/mol×K	1137.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390356&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