Succinic acid, 2,2,3,3-tetrafluoropropyl 2,4,6-trichlorophenyl ester

Inchi: InChI=1S/C13H9Cl3F4O4/c14-6-3-7(15)11(8(16)4-6)24-10(22)2-1-9(21)23-5-13(19,20)12

InchiKey: CYUPBYVKYVPYMU-UHFFFAOYSA-N

Formula: C13H9Cl3F4O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 411.56

Physical Properties

Property code	Value	Unit	Source
gf	-1140.37	kJ/mol	Joback Method
hf	-1444.82	kJ/mol	Joback Method
hfus	41.85	kJ/mol	Joback Method
hvap	75.31	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.776		Crippen Method
mcvol	228.950	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	2025.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	796.74	K	Joback Method
tc	1000.70	K	Joback Method
tf	524.11	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.39	J/mol×K	796.74	Joback Method
cpg	598.48	J/mol×K	830.73	Joback Method
cpg	606.78	J/mol×K	864.73	Joback Method
cpg	614.33	J/mol×K	898.72	Joback Method
cpg	621.13	J/mol×K	932.71	Joback Method
cpg	627.22	J/mol×K	966.70	Joback Method
cpg	632.61	J/mol×K	1000.70	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=U390268&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