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

Inchi: InChI=1S/C13H8Cl3F5O4/c14-6-3-7(15)11(8(16)4-6)25-10(23)2-1-9(22)24-5-12(17,18)13

InchiKey: GZNRJZLJASABCD-UHFFFAOYSA-N

Formula: C13H8Cl3F5O4

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

Mol. weight [g/mol]: 429.55

Physical Properties

Property code	Value	Unit	Source
gf	-1329.90	kJ/mol	Joback Method
hf	-1644.40	kJ/mol	Joback Method
hfus	41.04	kJ/mol	Joback Method
hvap	73.58	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.073		Crippen Method
mcvol	230.720	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1906.00		NIST Webbook
rinpol	1906.00		NIST Webbook
tb	793.22	K	Joback Method
tc	995.78	K	Joback Method
tf	542.12	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	598.70	J/mol×K	793.22	Joback Method
cpg	607.32	J/mol×K	826.98	Joback Method
cpg	615.19	J/mol×K	860.74	Joback Method
cpg	622.34	J/mol×K	894.50	Joback Method
cpg	628.82	J/mol×K	928.26	Joback Method
cpg	634.65	J/mol×K	962.02	Joback Method
cpg	639.89	J/mol×K	995.78	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=U390875&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