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

Inchi: InChI=1S/C16H8Cl3F3O4/c17-7-5-8(18)16(9(19)6-7)26-13(24)4-3-12(23)25-11-2-1-10(20

InchiKey: IWVWDAVTJCOBAV-UHFFFAOYSA-N

Formula: C16H8Cl3F3O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 427.59

Physical Properties

Property code	Value	Unit	Source
gf	-837.18	kJ/mol	Joback Method
hf	-1094.48	kJ/mol	Joback Method
hfus	50.35	kJ/mol	Joback Method
hvap	88.75	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.355		Crippen Method
mcvol	245.690	ml/mol	McGowan Method
pc	1832.54	kPa	Joback Method
rinpol	2565.00		NIST Webbook
rinpol	2565.00		NIST Webbook
tb	911.40	K	Joback Method
tc	1136.90	K	Joback Method
tf	633.89	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	633.71	J/mol×K	911.40	Joback Method
cpg	641.55	J/mol×K	948.98	Joback Method
cpg	648.37	J/mol×K	986.57	Joback Method
cpg	654.15	J/mol×K	1024.15	Joback Method
cpg	658.88	J/mol×K	1061.73	Joback Method
cpg	662.59	J/mol×K	1099.32	Joback Method
cpg	665.25	J/mol×K	1136.90	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=U390771&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

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