Succinic acid, 2,4,6-trichlorophenyl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C17H9Cl3F4O4/c18-8-6-10(19)16(11(20)7-8)28-14(26)5-4-13(25)27-12-3-1-2-9

InchiKey: JWXAVHPGLLIHSR-UHFFFAOYSA-N

Formula: C17H9Cl3F4O4

SMILES: O=C(CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 459.60

Physical Properties

Property code	Value	Unit	Source
gf	-1011.10	kJ/mol	Joback Method
hf	-1308.51	kJ/mol	Joback Method
hfus	48.99	kJ/mol	Joback Method
hvap	88.20	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	6.096		Crippen Method
mcvol	261.550	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	925.34	K	Joback Method
tc	1150.35	K	Joback Method
tf	635.65	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.87	J/mol×K	925.34	Joback Method
cpg	706.81	J/mol×K	962.84	Joback Method
cpg	713.78	J/mol×K	1000.34	Joback Method
cpg	719.81	J/mol×K	1037.85	Joback Method
cpg	724.94	J/mol×K	1075.35	Joback Method
cpg	729.20	J/mol×K	1112.85	Joback Method
cpg	732.62	J/mol×K	1150.35	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390793&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