Succinic acid, 4-chloro-3-methylphenyl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C18H13ClF4O4/c1-10-9-11(5-6-13(10)19)26-15(24)7-8-16(25)27-14-4-2-3-12(1

InchiKey: MOBJYMQPOQQWSC-UHFFFAOYSA-N

Formula: C18H13ClF4O4

SMILES: Cc1cc(OC(=O)CCC(=O)Oc2cccc(C(F)(F)F)c2F)ccc1Cl

Mol. weight [g/mol]: 404.74

Physical Properties

Property code	Value	Unit	Source
gf	-969.19	kJ/mol	Joback Method
hf	-1286.20	kJ/mol	Joback Method
hfus	43.58	kJ/mol	Joback Method
hvap	80.99	kJ/mol	Joback Method
log10ws	-6.34		Crippen Method
logp	5.098		Crippen Method
mcvol	251.160	ml/mol	McGowan Method
pc	1665.97	kPa	Joback Method
rinpol	2456.00		NIST Webbook
rinpol	2456.00		NIST Webbook
tb	868.38	K	Joback Method
tc	1083.67	K	Joback Method
tf	574.56	K	Joback Method
vc	0.986	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.75	J/mol×K	868.38	Joback Method
cpg	728.37	J/mol×K	904.26	Joback Method
cpg	737.97	J/mol×K	940.14	Joback Method
cpg	746.58	J/mol×K	976.03	Joback Method
cpg	754.26	J/mol×K	1011.91	Joback Method
cpg	761.02	J/mol×K	1047.79	Joback Method
cpg	766.90	J/mol×K	1083.67	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390790&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