Succinic acid, 3-chlorophenyl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C17H11ClF4O4/c18-10-3-1-4-11(9-10)25-14(23)7-8-15(24)26-13-6-2-5-12(16(1

InchiKey: QAOGCKUCBNQFEX-UHFFFAOYSA-N

Formula: C17H11ClF4O4

SMILES: O=C(CCC(=O)Oc1cccc(C(F)(F)F)c1F)Oc1cccc(Cl)c1

Mol. weight [g/mol]: 390.71

Physical Properties

Property code	Value	Unit	Source
gf	-967.98	kJ/mol	Joback Method
hf	-1254.09	kJ/mol	Joback Method
hfus	41.38	kJ/mol	Joback Method
hvap	78.11	kJ/mol	Joback Method
log10ws	-5.87		Crippen Method
logp	4.789		Crippen Method
mcvol	237.070	ml/mol	McGowan Method
pc	1827.85	kPa	Joback Method
rinpol	2306.00		NIST Webbook
rinpol	2306.00		NIST Webbook
tb	840.52	K	Joback Method
tc	1056.07	K	Joback Method
tf	550.77	K	Joback Method
vc	0.929	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.33	J/mol×K	840.52	Joback Method
cpg	674.75	J/mol×K	876.44	Joback Method
cpg	684.18	J/mol×K	912.37	Joback Method
cpg	692.66	J/mol×K	948.29	Joback Method
cpg	700.22	J/mol×K	984.22	Joback Method
cpg	706.91	J/mol×K	1020.14	Joback Method
cpg	712.76	J/mol×K	1056.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390788&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

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