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

Inchi: InChI=1S/C18H10F8O4/c19-15-9(17(21,22)23)3-1-5-11(15)29-13(27)7-8-14(28)30-12-6-

InchiKey: NOKUJWOOTMHONP-UHFFFAOYSA-N

Formula: C18H10F8O4

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

Mol. weight [g/mol]: 442.26

Physical Properties

Property code	Value	Unit	Source
gf	-1733.66	kJ/mol	Joback Method
hf	-2063.65	kJ/mol	Joback Method
hfus	44.29	kJ/mol	Joback Method
hvap	72.05	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.294		Crippen Method
mcvol	246.000	ml/mol	McGowan Method
pc	1509.33	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook
tb	824.80	K	Joback Method
tc	1021.78	K	Joback Method
tf	549.42	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.74	J/mol×K	824.80	Joback Method
cpg	738.09	J/mol×K	857.63	Joback Method
cpg	747.55	J/mol×K	890.46	Joback Method
cpg	756.17	J/mol×K	923.29	Joback Method
cpg	763.99	J/mol×K	956.12	Joback Method
cpg	771.07	J/mol×K	988.95	Joback Method
cpg	777.44	J/mol×K	1021.78	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=U390796&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