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

Inchi: InChI=1S/C17H11F5O4/c18-11-5-1-2-6-12(11)25-14(23)8-9-15(24)26-13-7-3-4-10(16(13

InchiKey: CKONCZCGDYNTOE-UHFFFAOYSA-N

Formula: C17H11F5O4

SMILES: O=C(CCC(=O)Oc1cccc(C(F)(F)F)c1F)Oc1ccccc1F

Mol. weight [g/mol]: 374.26

Physical Properties

Property code	Value	Unit	Source
gf	-1150.86	kJ/mol	Joback Method
hf	-1434.46	kJ/mol	Joback Method
hfus	40.26	kJ/mol	Joback Method
hvap	72.91	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.275		Crippen Method
mcvol	226.600	ml/mol	McGowan Method
pc	1815.41	kPa	Joback Method
rinpol	2116.00		NIST Webbook
rinpol	2116.00		NIST Webbook
tb	802.36	K	Joback Method
tc	1007.90	K	Joback Method
tf	521.44	K	Joback Method
vc	0.898	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.16	J/mol×K	802.36	Joback Method
cpg	661.33	J/mol×K	836.62	Joback Method
cpg	671.54	J/mol×K	870.87	Joback Method
cpg	680.84	J/mol×K	905.13	Joback Method
cpg	689.25	J/mol×K	939.39	Joback Method
cpg	696.81	J/mol×K	973.64	Joback Method
cpg	703.55	J/mol×K	1007.90	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=U390784&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