Succinic acid, 2,2,3,3-tetrafluoropropyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C13H9F7O4/c14-6-1-2-7(11(16)10(6)15)24-9(22)4-3-8(21)23-5-13(19,20)12(17

InchiKey: MQEOLGLKLUCORE-UHFFFAOYSA-N

Formula: C13H9F7O4

SMILES: O=C(CCC(=O)Oc1ccc(F)c(F)c1F)OCC(F)(F)C(F)F

Mol. weight [g/mol]: 362.20

Physical Properties

Property code	Value	Unit	Source
gf	-1689.01	kJ/mol	Joback Method
hf	-1985.93	kJ/mol	Joback Method
hfus	38.50	kJ/mol	Joback Method
hvap	59.70	kJ/mol	Joback Method
log10ws	-4.36		Crippen Method
logp	3.233		Crippen Method
mcvol	197.540	ml/mol	McGowan Method
pc	1771.36	kPa	Joback Method
rinpol	1630.00		NIST Webbook
rinpol	1630.00		NIST Webbook
tb	682.26	K	Joback Method
tc	856.36	K	Joback Method
tf	436.12	K	Joback Method
vc	0.812	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.96	J/mol×K	682.26	Joback Method
cpg	555.63	J/mol×K	711.28	Joback Method
cpg	565.67	J/mol×K	740.29	Joback Method
cpg	575.07	J/mol×K	769.31	Joback Method
cpg	583.87	J/mol×K	798.33	Joback Method
cpg	592.06	J/mol×K	827.34	Joback Method
cpg	599.65	J/mol×K	856.36	Joback Method

Sources

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=U390754&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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