Succinic acid, 1,1,1-trifluoroprop-2-yl 2-isopropoxyphenyl ester

Inchi: InChI=1S/C16H19F3O5/c1-10(2)22-12-6-4-5-7-13(12)24-15(21)9-8-14(20)23-11(3)16(17
InchiKey: FYNDKOJCKNSEPL-UHFFFAOYSA-N
Formula: C16H19F3O5
SMILES: CC(C)Oc1ccccc1OC(=O)CCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 348.31

Physical Properties

Property code	Value	Unit	Source
gf	-972.69	kJ/mol	Joback Method
hf	-1377.97	kJ/mol	Joback Method
hfus	32.39	kJ/mol	Joback Method
hvap	70.35	kJ/mol	Joback Method
log10ws	-4.58		Crippen Method
logp	3.653		Crippen Method
mcvol	238.600	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	765.84	K	Joback Method
tc	961.27	K	Joback Method
tf	449.76	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.37	J/mol×K	765.84	Joback Method
cpg	716.19	J/mol×K	798.41	Joback Method
cpg	729.03	J/mol×K	830.98	Joback Method
cpg	740.90	J/mol×K	863.55	Joback Method
cpg	751.82	J/mol×K	896.12	Joback Method
cpg	761.81	J/mol×K	928.70	Joback Method
cpg	770.89	J/mol×K	961.27	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=U389783&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