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

Inchi: InChI=1S/C16H19F3O4/c1-3-6-12-7-4-5-8-13(12)23-15(21)10-9-14(20)22-11(2)16(17,18

InchiKey: FNYZOAUHXBDWJF-UHFFFAOYSA-N

Formula: C16H19F3O4

SMILES: CCCc1ccccc1OC(=O)CCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 332.31

Physical Properties

Property code	Value	Unit	Source
gf	-865.25	kJ/mol	Joback Method
hf	-1240.47	kJ/mol	Joback Method
hfus	34.72	kJ/mol	Joback Method
hvap	68.33	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	3.819		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1660.55	kPa	Joback Method
rinpol	1735.00		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	743.86	K	Joback Method
tc	936.95	K	Joback Method
tf	442.53	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.38	J/mol×K	743.86	Joback Method
cpg	688.37	J/mol×K	776.04	Joback Method
cpg	701.42	J/mol×K	808.22	Joback Method
cpg	713.57	J/mol×K	840.41	Joback Method
cpg	724.85	J/mol×K	872.59	Joback Method
cpg	735.28	J/mol×K	904.77	Joback Method
cpg	744.90	J/mol×K	936.95	Joback Method

Sources

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=U390383&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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