Succinic acid, 1,1,1-trifluoroprop-2-yl 4-biphenyl ester

Inchi: InChI=1S/C19H17F3O4/c1-13(19(20,21)22)25-17(23)11-12-18(24)26-16-9-7-15(8-10-16)

InchiKey: NQDRJQVMFGYVFN-UHFFFAOYSA-N

Formula: C19H17F3O4

SMILES: CC(OC(=O)CCC(=O)Oc1ccc(-c2ccccc2)cc1)C(F)(F)F

Mol. weight [g/mol]: 366.33

Physical Properties

Property code	Value	Unit	Source
gf	-727.58	kJ/mol	Joback Method
hf	-1065.86	kJ/mol	Joback Method
hfus	36.54	kJ/mol	Joback Method
hvap	77.28	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	4.533		Crippen Method
mcvol	251.240	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2380.00		NIST Webbook
rinpol	2380.00		NIST Webbook
tb	839.18	K	Joback Method
tc	1055.66	K	Joback Method
tf	502.76	K	Joback Method
vc	0.969	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	748.70	J/mol×K	839.18	Joback Method
cpg	761.60	J/mol×K	875.26	Joback Method
cpg	773.35	J/mol×K	911.34	Joback Method
cpg	784.02	J/mol×K	947.42	Joback Method
cpg	793.65	J/mol×K	983.50	Joback Method
cpg	802.30	J/mol×K	1019.58	Joback Method
cpg	810.03	J/mol×K	1055.66	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=U390078&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