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

Inchi: InChI=1S/C20H19F3O4/c1-14(20(21,22)23)26-17(24)12-13-18(25)27-19(15-8-4-2-5-9-15

InchiKey: HVRXSILVVGKWHK-UHFFFAOYSA-N

Formula: C20H19F3O4

SMILES: CC(OC(=O)CCC(=O)OC(c1ccccc1)c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 380.36

Physical Properties

Property code	Value	Unit	Source
gf	-711.97	kJ/mol	Joback Method
hf	-1080.31	kJ/mol	Joback Method
hfus	35.99	kJ/mol	Joback Method
hvap	78.46	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.593		Crippen Method
mcvol	265.330	ml/mol	McGowan Method
pc	1620.68	kPa	Joback Method
rinpol	2180.00		NIST Webbook
rinpol	2180.00		NIST Webbook
tb	856.64	K	Joback Method
tc	1073.66	K	Joback Method
tf	486.51	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	806.96	J/mol×K	856.64	Joback Method
cpg	820.26	J/mol×K	892.81	Joback Method
cpg	832.36	J/mol×K	928.98	Joback Method
cpg	843.33	J/mol×K	965.15	Joback Method
cpg	853.23	J/mol×K	1001.32	Joback Method
cpg	862.15	J/mol×K	1037.49	Joback Method
cpg	870.13	J/mol×K	1073.66	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=U390162&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