Succinic acid, di(1-phenyl-2,2,2-trifluoroethyl) ester

Inchi: InChI=1S/C20H16F6O4/c21-19(22,23)17(13-7-3-1-4-8-13)29-15(27)11-12-16(28)30-18(2

InchiKey: KWZQDZZHVIDKIU-UHFFFAOYSA-N

Formula: C20H16F6O4

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

Mol. weight [g/mol]: 434.33

Physical Properties

Property code	Value	Unit	Source
gf	-1293.56	kJ/mol	Joback Method
hf	-1677.39	kJ/mol	Joback Method
hfus	37.82	kJ/mol	Joback Method
hvap	74.71	kJ/mol	Joback Method
log10ws	-6.37		Crippen Method
logp	5.460		Crippen Method
mcvol	270.640	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	2052.00		NIST Webbook
rinpol	2052.00		NIST Webbook
tb	851.22	K	Joback Method
tc	1058.30	K	Joback Method
tf	490.70	K	Joback Method
vc	1.062	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	830.43	J/mol×K	851.22	Joback Method
cpg	842.57	J/mol×K	885.73	Joback Method
cpg	853.64	J/mol×K	920.25	Joback Method
cpg	863.72	J/mol×K	954.76	Joback Method
cpg	872.89	J/mol×K	989.27	Joback Method
cpg	881.24	J/mol×K	1023.78	Joback Method
cpg	888.85	J/mol×K	1058.30	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=U381584&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