Succinic acid, 2,2,3,3-tetrafluoropropyl diphenylmethyl ester

Inchi: InChI=1S/C20H18F4O4/c21-19(22)20(23,24)13-27-16(25)11-12-17(26)28-18(14-7-3-1-4-

InchiKey: FLSPSGZPJVWEIH-UHFFFAOYSA-N

Formula: C20H18F4O4

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

Mol. weight [g/mol]: 398.35

Physical Properties

Property code	Value	Unit	Source
gf	-906.78	kJ/mol	Joback Method
hf	-1276.42	kJ/mol	Joback Method
hfus	39.07	kJ/mol	Joback Method
hvap	77.64	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.543		Crippen Method
mcvol	267.100	ml/mol	McGowan Method
pc	1563.52	kPa	Joback Method
rinpol	2273.00		NIST Webbook
rinpol	2273.00		NIST Webbook
tb	855.91	K	Joback Method
tc	1067.23	K	Joback Method
tf	487.10	K	Joback Method
vc	1.036	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	814.35	J/mol×K	855.91	Joback Method
cpg	827.19	J/mol×K	891.13	Joback Method
cpg	838.90	J/mol×K	926.35	Joback Method
cpg	849.52	J/mol×K	961.57	Joback Method
cpg	859.13	J/mol×K	996.79	Joback Method
cpg	867.80	J/mol×K	1032.01	Joback Method
cpg	875.57	J/mol×K	1067.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390163&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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