Succinic acid, decyl 1-phenyl-2,2,2-trifluoroethyl ester

Inchi: InChI=1S/C22H31F3O4/c1-2-3-4-5-6-7-8-12-17-28-19(26)15-16-20(27)29-21(22(23,24)2

InchiKey: JTYYVKHWNADPRB-UHFFFAOYSA-N

Formula: C22H31F3O4

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

Mol. weight [g/mol]: 416.47

Physical Properties

Property code	Value	Unit	Source
gf	-805.10	kJ/mol	Joback Method
hf	-1352.84	kJ/mol	Joback Method
hfus	50.65	kJ/mol	Joback Method
hvap	81.02	kJ/mol	Joback Method
log10ws	-6.98		Crippen Method
logp	6.297		Crippen Method
mcvol	317.270	ml/mol	McGowan Method
pc	1100.08	kPa	Joback Method
rinpol	2387.00		NIST Webbook
rinpol	2387.00		NIST Webbook
tb	876.16	K	Joback Method
tc	1074.69	K	Joback Method
tf	497.63	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.57	J/mol×K	876.16	Joback Method
cpg	1036.39	J/mol×K	909.25	Joback Method
cpg	1051.07	J/mol×K	942.34	Joback Method
cpg	1064.65	J/mol×K	975.42	Joback Method
cpg	1077.19	J/mol×K	1008.51	Joback Method
cpg	1088.74	J/mol×K	1041.60	Joback Method
cpg	1099.34	J/mol×K	1074.69	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=U381577&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