Sebacic acid, isobutyl 1-phenyl-2,2,2-trifluoromethylethyl ester

Inchi: InChI=1S/C22H31F3O4/c1-17(2)16-28-19(26)14-10-5-3-4-6-11-15-20(27)29-21(22(23,24

InchiKey: KCCNIUVRWWHLML-UHFFFAOYSA-N

Formula: C22H31F3O4

SMILES: CC(C)COC(=O)CCCCCCCCC(=O)OC(c1ccccc1)C(F)(F)F

Mol. weight [g/mol]: 416.47

Physical Properties

Property code	Value	Unit	Source
gf	-807.54	kJ/mol	Joback Method
hf	-1358.12	kJ/mol	Joback Method
hfus	47.13	kJ/mol	Joback Method
hvap	80.63	kJ/mol	Joback Method
log10ws	-6.74		Crippen Method
logp	6.153		Crippen Method
mcvol	317.270	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
rinpol	2304.00		NIST Webbook
rinpol	2304.00		NIST Webbook
tb	875.72	K	Joback Method
tc	1074.97	K	Joback Method
tf	482.63	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1021.06	J/mol×K	875.72	Joback Method
cpg	1036.92	J/mol×K	908.93	Joback Method
cpg	1051.62	J/mol×K	942.14	Joback Method
cpg	1065.20	J/mol×K	975.35	Joback Method
cpg	1077.73	J/mol×K	1008.56	Joback Method
cpg	1089.24	J/mol×K	1041.76	Joback Method
cpg	1099.79	J/mol×K	1074.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416801&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