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

Inchi: InChI=1S/C31H49F3O4/c1-2-3-4-5-6-7-8-9-12-15-21-26-37-28(35)24-19-13-10-11-14-20
InchiKey: KZSORXBBJNIABT-UHFFFAOYSA-N
Formula: C31H49F3O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(c1ccccc1)C(F)(F)F
Mol. weight [g/mol]: 542.71

Physical Properties

Property code	Value	Unit	Source
gf	-729.32	kJ/mol	Joback Method
hf	-1538.60	kJ/mol	Joback Method
hfus	73.96	kJ/mol	Joback Method
hvap	101.05	kJ/mol	Joback Method
log10ws	-10.75		Crippen Method
logp	9.808		Crippen Method
mcvol	444.080	ml/mol	McGowan Method
pc	664.60	kPa	Joback Method
rinpol	3093.00		NIST Webbook
rinpol	3093.00		NIST Webbook
tb	1082.08	K	Joback Method
tc	1353.16	K	Joback Method
tf	599.06	K	Joback Method
vc	1.748	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1581.01	J/mol×K	1082.08	Joback Method
cpg	1601.28	J/mol×K	1127.26	Joback Method
cpg	1619.53	J/mol×K	1172.44	Joback Method
cpg	1635.94	J/mol×K	1217.62	Joback Method
cpg	1650.71	J/mol×K	1262.80	Joback Method
cpg	1664.02	J/mol×K	1307.98	Joback Method
cpg	1676.06	J/mol×K	1353.16	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416810&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