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

Inchi: InChI=1S/C32H51F3O4/c1-2-3-4-5-6-7-8-9-10-13-16-22-27-38-29(36)25-20-14-11-12-15
InchiKey: DIHHCOZELFEVDZ-UHFFFAOYSA-N
Formula: C32H51F3O4
SMILES: CCCCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(c1ccccc1)C(F)(F)F
Mol. weight [g/mol]: 556.74

Physical Properties

Property code	Value	Unit	Source
gf	-720.90	kJ/mol	Joback Method
hf	-1559.24	kJ/mol	Joback Method
hfus	76.55	kJ/mol	Joback Method
hvap	103.28	kJ/mol	Joback Method
log10ws	-11.17		Crippen Method
logp	10.198		Crippen Method
mcvol	458.170	ml/mol	McGowan Method
pc	632.89	kPa	Joback Method
rinpol	3155.00		NIST Webbook
rinpol	3155.00		NIST Webbook
tb	1104.96	K	Joback Method
tc	1391.00	K	Joback Method
tf	610.33	K	Joback Method
vc	1.804	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1645.24	J/mol×K	1104.96	Joback Method
cpg	1666.31	J/mol×K	1152.63	Joback Method
cpg	1685.18	J/mol×K	1200.31	Joback Method
cpg	1702.09	J/mol×K	1247.98	Joback Method
cpg	1717.26	J/mol×K	1295.65	Joback Method
cpg	1730.93	J/mol×K	1343.32	Joback Method
cpg	1743.32	J/mol×K	1391.00	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=U416811&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