Sebacic acid, di(1-phenyl-2,2,2-trifluoromethylethyl) ester

Inchi: InChI=1S/C26H28F6O4/c27-25(28,29)23(19-13-7-5-8-14-19)35-21(33)17-11-3-1-2-4-12-

InchiKey: PIMLFEBSXKKYCL-UHFFFAOYSA-N

Formula: C26H28F6O4

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

Mol. weight [g/mol]: 518.49

Physical Properties

Property code	Value	Unit	Source
gf	-1243.04	kJ/mol	Joback Method
hf	-1801.23	kJ/mol	Joback Method
hfus	53.36	kJ/mol	Joback Method
hvap	88.06	kJ/mol	Joback Method
log10ws	-8.88		Crippen Method
logp	7.801		Crippen Method
mcvol	355.180	ml/mol	McGowan Method
pc	991.38	kPa	Joback Method
tb	988.50	K	Joback Method
tc	1210.21	K	Joback Method
tf	558.32	K	Joback Method
vc	1.397	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1180.72	J/mol×K	988.50	Joback Method
cpg	1194.44	J/mol×K	1025.45	Joback Method
cpg	1207.03	J/mol×K	1062.40	Joback Method
cpg	1218.60	J/mol×K	1099.35	Joback Method
cpg	1229.26	J/mol×K	1136.30	Joback Method
cpg	1239.15	J/mol×K	1173.25	Joback Method
cpg	1248.37	J/mol×K	1210.21	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416814&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume