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

Inchi: InChI=1S/C30H47F3O4/c1-2-3-4-5-6-7-8-11-14-20-25-36-27(34)23-18-12-9-10-13-19-24
InchiKey: CFQYGRDOXSXXKY-UHFFFAOYSA-N
Formula: C30H47F3O4
SMILES: CCCCCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(c1ccccc1)C(F)(F)F
Mol. weight [g/mol]: 528.69

Physical Properties

Property code	Value	Unit	Source
gf	-737.74	kJ/mol	Joback Method
hf	-1517.96	kJ/mol	Joback Method
hfus	71.37	kJ/mol	Joback Method
hvap	98.83	kJ/mol	Joback Method
log10ws	-10.33		Crippen Method
logp	9.418		Crippen Method
mcvol	429.990	ml/mol	McGowan Method
pc	698.76	kPa	Joback Method
rinpol	3038.00		NIST Webbook
rinpol	3038.00		NIST Webbook
tb	1059.20	K	Joback Method
tc	1316.98	K	Joback Method
tf	587.79	K	Joback Method
vc	1.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1517.09	J/mol×K	1059.20	Joback Method
cpg	1536.64	J/mol×K	1102.16	Joback Method
cpg	1554.32	J/mol×K	1145.13	Joback Method
cpg	1570.29	J/mol×K	1188.09	Joback Method
cpg	1584.70	J/mol×K	1231.06	Joback Method
cpg	1597.71	J/mol×K	1274.02	Joback Method
cpg	1609.48	J/mol×K	1316.98	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=U416809&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