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

Inchi: InChI=1S/C28H43F3O4/c1-2-3-4-5-6-9-12-18-23-34-25(32)21-16-10-7-8-11-17-22-26(33

InchiKey: KSNNTHAWNWCNOY-UHFFFAOYSA-N

Formula: C28H43F3O4

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

Mol. weight [g/mol]: 500.63

Physical Properties

Property code	Value	Unit	Source
gf	-754.58	kJ/mol	Joback Method
hf	-1476.68	kJ/mol	Joback Method
hfus	66.19	kJ/mol	Joback Method
hvap	94.37	kJ/mol	Joback Method
log10ws	-9.49		Crippen Method
logp	8.638		Crippen Method
mcvol	401.810	ml/mol	McGowan Method
pc	775.48	kPa	Joback Method
rinpol	2868.00		NIST Webbook
rinpol	2868.00		NIST Webbook
tb	1013.44	K	Joback Method
tc	1249.15	K	Joback Method
tf	565.25	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1390.26	J/mol×K	1013.44	Joback Method
cpg	1408.58	J/mol×K	1052.73	Joback Method
cpg	1425.28	J/mol×K	1092.01	Joback Method
cpg	1440.48	J/mol×K	1131.30	Joback Method
cpg	1454.29	J/mol×K	1170.58	Joback Method
cpg	1466.83	J/mol×K	1209.87	Joback Method
cpg	1478.20	J/mol×K	1249.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416807&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume