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

Inchi: InChI=1S/C24H35F3O4/c1-2-3-4-14-19-30-21(28)17-12-7-5-6-8-13-18-22(29)31-23(24(2

InchiKey: WVXUEBPKDFYPCD-UHFFFAOYSA-N

Formula: C24H35F3O4

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

Mol. weight [g/mol]: 444.53

Physical Properties

Property code	Value	Unit	Source
gf	-788.26	kJ/mol	Joback Method
hf	-1394.12	kJ/mol	Joback Method
hfus	55.83	kJ/mol	Joback Method
hvap	85.47	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	7.077		Crippen Method
mcvol	345.450	ml/mol	McGowan Method
pc	972.30	kPa	Joback Method
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
tb	921.92	K	Joback Method
tc	1128.69	K	Joback Method
tf	520.17	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1141.67	J/mol×K	921.92	Joback Method
cpg	1158.16	J/mol×K	956.38	Joback Method
cpg	1173.40	J/mol×K	990.84	Joback Method
cpg	1187.44	J/mol×K	1025.31	Joback Method
cpg	1200.35	J/mol×K	1059.77	Joback Method
cpg	1212.18	J/mol×K	1094.23	Joback Method
cpg	1223.02	J/mol×K	1128.69	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=U416804&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