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

Inchi: InChI=1S/C34H55F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-24-29-40-31(38)27-22-16-13

InchiKey: YIBJRSRZGIFPAQ-UHFFFAOYSA-N

Formula: C34H55F3O4

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

Mol. weight [g/mol]: 584.79

Physical Properties

Property code	Value	Unit	Source
gf	-704.06	kJ/mol	Joback Method
hf	-1600.52	kJ/mol	Joback Method
hfus	81.73	kJ/mol	Joback Method
hvap	107.73	kJ/mol	Joback Method
log10ws	-12.00		Crippen Method
logp	10.979		Crippen Method
mcvol	486.350	ml/mol	McGowan Method
pc	575.91	kPa	Joback Method
rinpol	3325.00		NIST Webbook
tb	1150.72	K	Joback Method
tc	1472.24	K	Joback Method
tf	632.87	K	Joback Method
vc	1.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1774.52	J/mol×K	1150.72	Joback Method
cpg	1797.44	J/mol×K	1204.31	Joback Method
cpg	1817.78	J/mol×K	1257.89	Joback Method
cpg	1835.87	J/mol×K	1311.48	Joback Method
cpg	1852.07	J/mol×K	1365.07	Joback Method
cpg	1866.73	J/mol×K	1418.65	Joback Method
cpg	1880.21	J/mol×K	1472.24	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=U416813&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