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

Inchi: InChI=1S/C33H53F3O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-23-28-39-30(37)26-21-15-12-13

InchiKey: VWSDPZVYLPTGPL-UHFFFAOYSA-N

Formula: C33H53F3O4

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

Mol. weight [g/mol]: 570.77

Physical Properties

Property code	Value	Unit	Source
gf	-712.48	kJ/mol	Joback Method
hf	-1579.88	kJ/mol	Joback Method
hfus	79.14	kJ/mol	Joback Method
hvap	105.50	kJ/mol	Joback Method
log10ws	-11.59		Crippen Method
logp	10.588		Crippen Method
mcvol	472.260	ml/mol	McGowan Method
pc	603.39	kPa	Joback Method
rinpol	3231.00		NIST Webbook
rinpol	3231.00		NIST Webbook
tb	1127.84	K	Joback Method
tc	1430.64	K	Joback Method
tf	621.60	K	Joback Method
vc	1.861	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1709.75	J/mol×K	1127.84	Joback Method
cpg	1731.70	J/mol×K	1178.31	Joback Method
cpg	1751.26	J/mol×K	1228.77	Joback Method
cpg	1768.72	J/mol×K	1279.24	Joback Method
cpg	1784.37	J/mol×K	1329.71	Joback Method
cpg	1798.48	J/mol×K	1380.17	Joback Method
cpg	1811.33	J/mol×K	1430.64	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=U416812&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