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

Inchi: InChI=1S/C26H39F3O4/c1-2-3-4-5-10-16-21-32-23(30)19-14-8-6-7-9-15-20-24(31)33-25

InchiKey: XRNQLQOVXYAXLB-UHFFFAOYSA-N

Formula: C26H39F3O4

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

Mol. weight [g/mol]: 472.58

Physical Properties

Property code	Value	Unit	Source
gf	-771.42	kJ/mol	Joback Method
hf	-1435.40	kJ/mol	Joback Method
hfus	61.01	kJ/mol	Joback Method
hvap	89.92	kJ/mol	Joback Method
log10ws	-8.66		Crippen Method
logp	7.858		Crippen Method
mcvol	373.630	ml/mol	McGowan Method
pc	865.56	kPa	Joback Method
rinpol	2693.00		NIST Webbook
rinpol	2693.00		NIST Webbook
tb	967.68	K	Joback Method
tc	1186.64	K	Joback Method
tf	542.71	K	Joback Method
vc	1.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1265.02	J/mol×K	967.68	Joback Method
cpg	1282.33	J/mol×K	1004.17	Joback Method
cpg	1298.23	J/mol×K	1040.67	Joback Method
cpg	1312.80	J/mol×K	1077.16	Joback Method
cpg	1326.12	J/mol×K	1113.65	Joback Method
cpg	1338.28	J/mol×K	1150.14	Joback Method
cpg	1349.36	J/mol×K	1186.64	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=U416806&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