Phthalic acid, 2,2,2-trifluoro-1-phenylethyl undecyl ester

Inchi: InChI=1S/C27H33F3O4/c1-2-3-4-5-6-7-8-9-15-20-33-25(31)22-18-13-14-19-23(22)26(32
InchiKey: KLOBUMUNUSSNII-UHFFFAOYSA-N
Formula: C27H33F3O4
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OC(c1ccccc1)C(F)(F)F
Mol. weight [g/mol]: 478.54

Physical Properties

Property code	Value	Unit	Source
gf	-660.22	kJ/mol	Joback Method
hf	-1230.98	kJ/mol	Joback Method
hfus	57.26	kJ/mol	Joback Method
hvap	95.09	kJ/mol	Joback Method
log10ws	-9.30		Crippen Method
logp	7.835		Crippen Method
mcvol	363.960	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinpol	2898.00		NIST Webbook
rinpol	2898.00		NIST Webbook
tb	1022.22	K	Joback Method
tc	1251.50	K	Joback Method
tf	592.92	K	Joback Method
vc	1.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1219.44	J/mol×K	1022.22	Joback Method
cpg	1233.78	J/mol×K	1060.43	Joback Method
cpg	1246.77	J/mol×K	1098.65	Joback Method
cpg	1258.51	J/mol×K	1136.86	Joback Method
cpg	1269.10	J/mol×K	1175.07	Joback Method
cpg	1278.64	J/mol×K	1213.29	Joback Method
cpg	1287.23	J/mol×K	1251.50	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=U377709&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