Phthalic acid, 4-trifluoromethoxybenzyl undecyl ester

Inchi: InChI=1S/C27H33F3O5/c1-2-3-4-5-6-7-8-9-12-19-33-25(31)23-13-10-11-14-24(23)26(32
InchiKey: ZOLPZHCGWFVMAC-UHFFFAOYSA-N
Formula: C27H33F3O5
SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1ccc(OC(F)(F)F)cc1
Mol. weight [g/mol]: 494.54

Physical Properties

Property code	Value	Unit	Source
gf	-772.41	kJ/mol	Joback Method
hf	-1369.39	kJ/mol	Joback Method
hfus	61.58	kJ/mol	Joback Method
hvap	98.55	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	7.630		Crippen Method
mcvol	369.830	ml/mol	McGowan Method
pc	965.07	kPa	Joback Method
rinpol	2989.00		NIST Webbook
rinpol	2989.00		NIST Webbook
tb	1050.06	K	Joback Method
tc	1286.87	K	Joback Method
tf	642.67	K	Joback Method
vc	1.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1244.61	J/mol×K	1050.06	Joback Method
cpg	1257.86	J/mol×K	1089.53	Joback Method
cpg	1269.52	J/mol×K	1129.00	Joback Method
cpg	1279.66	J/mol×K	1168.46	Joback Method
cpg	1288.36	J/mol×K	1207.93	Joback Method
cpg	1295.71	J/mol×K	1247.40	Joback Method
cpg	1301.77	J/mol×K	1286.87	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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