Phthalic acid, 2,3,4,5-tetrafluorobenzyl undecyl ester

Inchi: InChI=1S/C26H30F4O4/c1-2-3-4-5-6-7-8-9-12-15-33-25(31)19-13-10-11-14-20(19)26(32

InchiKey: FISHFIFAFNKNBD-UHFFFAOYSA-N

Formula: C26H30F4O4

SMILES: CCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 482.51

Physical Properties

Property code	Value	Unit	Source
gf	-902.37	kJ/mol	Joback Method
hf	-1438.30	kJ/mol	Joback Method
hfus	67.13	kJ/mol	Joback Method
hvap	96.38	kJ/mol	Joback Method
log10ws	-9.58		Crippen Method
logp	7.288		Crippen Method
mcvol	351.640	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
rinpol	2924.00		NIST Webbook
tb	1022.20	K	Joback Method
tc	1253.30	K	Joback Method
tf	644.90	K	Joback Method
vc	1.395	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1160.22	J/mol×K	1022.20	Joback Method
cpg	1173.60	J/mol×K	1060.72	Joback Method
cpg	1185.36	J/mol×K	1099.23	Joback Method
cpg	1195.55	J/mol×K	1137.75	Joback Method
cpg	1204.21	J/mol×K	1176.26	Joback Method
cpg	1211.38	J/mol×K	1214.78	Joback Method
cpg	1217.10	J/mol×K	1253.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377734&Units=SI

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