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

Inchi: InChI=1S/C27H32F4O4/c1-2-3-4-5-6-7-8-9-10-13-16-34-26(32)20-14-11-12-15-21(20)27

InchiKey: IJINWXMTIYHXKO-UHFFFAOYSA-N

Formula: C27H32F4O4

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

Mol. weight [g/mol]: 496.53

Physical Properties

Property code	Value	Unit	Source
gf	-893.95	kJ/mol	Joback Method
hf	-1458.94	kJ/mol	Joback Method
hfus	69.72	kJ/mol	Joback Method
hvap	98.60	kJ/mol	Joback Method
log10ws	-10.00		Crippen Method
logp	7.678		Crippen Method
mcvol	365.730	ml/mol	McGowan Method
pc	912.18	kPa	Joback Method
rinpol	3025.00		NIST Webbook
rinpol	3025.00		NIST Webbook
tb	1045.08	K	Joback Method
tc	1283.97	K	Joback Method
tf	656.17	K	Joback Method
vc	1.452	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1220.91	J/mol×K	1045.08	Joback Method
cpg	1234.49	J/mol×K	1084.90	Joback Method
cpg	1246.33	J/mol×K	1124.71	Joback Method
cpg	1256.47	J/mol×K	1164.53	Joback Method
cpg	1264.97	J/mol×K	1204.34	Joback Method
cpg	1271.87	J/mol×K	1244.16	Joback Method
cpg	1277.21	J/mol×K	1283.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377735&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

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