Phthalic acid, pentafluorophenyl tetradecyl ester

Inchi: InChI=1S/C28H33F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-15-18-36-27(34)19-16-13-14-17-20
InchiKey: XFRJTXVMAKMMFD-UHFFFAOYSA-N
Formula: C28H33F5O4
SMILES: CCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 528.55

Physical Properties

Property code	Value	Unit	Source
gf	-1089.97	kJ/mol	Joback Method
hf	-1687.16	kJ/mol	Joback Method
hfus	75.00	kJ/mol	Joback Method
hvap	100.67	kJ/mol	Joback Method
log10ws	-10.90		Crippen Method
logp	8.459		Crippen Method
mcvol	381.590	ml/mol	McGowan Method
pc	831.94	kPa	Joback Method
rinpol	3047.00		NIST Webbook
tb	1072.21	K	Joback Method
tc	1325.72	K	Joback Method
tf	680.55	K	Joback Method
vc	1.526	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1287.11	J/mol×K	1072.21	Joback Method
cpg	1300.73	J/mol×K	1114.46	Joback Method
cpg	1312.33	J/mol×K	1156.71	Joback Method
cpg	1321.95	J/mol×K	1198.96	Joback Method
cpg	1329.66	J/mol×K	1241.21	Joback Method
cpg	1335.51	J/mol×K	1283.46	Joback Method
cpg	1339.55	J/mol×K	1325.72	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=U356363&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