Phthalic acid, pentafluorophenyl tridecyl ester

Inchi: InChI=1S/C27H31F5O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-35-26(33)18-15-12-13-16-19(18
InchiKey: BOXJJYUCXNCTRR-UHFFFAOYSA-N
Formula: C27H31F5O4
SMILES: CCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 514.52

Physical Properties

Property code	Value	Unit	Source
gf	-1098.39	kJ/mol	Joback Method
hf	-1666.52	kJ/mol	Joback Method
hfus	72.41	kJ/mol	Joback Method
hvap	98.45	kJ/mol	Joback Method
log10ws	-10.48		Crippen Method
logp	8.069		Crippen Method
mcvol	367.500	ml/mol	McGowan Method
pc	880.00	kPa	Joback Method
rinpol	2935.00		NIST Webbook
rinpol	2935.00		NIST Webbook
tb	1049.33	K	Joback Method
tc	1292.58	K	Joback Method
tf	669.28	K	Joback Method
vc	1.470	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1226.24	J/mol×K	1049.33	Joback Method
cpg	1239.64	J/mol×K	1089.87	Joback Method
cpg	1251.19	J/mol×K	1130.41	Joback Method
cpg	1260.94	J/mol×K	1170.96	Joback Method
cpg	1268.93	J/mol×K	1211.50	Joback Method
cpg	1275.22	J/mol×K	1252.04	Joback Method
cpg	1279.83	J/mol×K	1292.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356358&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