Phthalic acid, di(2,3,4,5-tetrafluorobenzyl) ester

Inchi: InChI=1S/C22H10F8O4/c23-13-5-9(15(25)19(29)17(13)27)7-33-21(31)11-3-1-2-4-12(11)
InchiKey: FDRYEBRGYQDRAN-UHFFFAOYSA-N
Formula: C22H10F8O4
SMILES: O=C(OCc1cc(F)c(F)c(F)c1F)c1ccccc1C(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]: 490.30

Physical Properties

Property code	Value	Unit	Source
gf	-1641.40	kJ/mol	Joback Method
hf	-1949.53	kJ/mol	Joback Method
hfus	61.57	kJ/mol	Joback Method
hvap	89.13	kJ/mol	Joback Method
log10ws	-8.83		Crippen Method
logp	5.513		Crippen Method
mcvol	278.600	ml/mol	McGowan Method
pc	1331.98	kPa	Joback Method
rinpol	2513.00		NIST Webbook
rinpol	2513.00		NIST Webbook
tb	974.36	K	Joback Method
tc	1193.84	K	Joback Method
tf	678.68	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.94	J/mol×K	974.36	Joback Method
cpg	845.38	J/mol×K	1010.94	Joback Method
cpg	852.56	J/mol×K	1047.52	Joback Method
cpg	858.47	J/mol×K	1084.10	Joback Method
cpg	863.13	J/mol×K	1120.68	Joback Method
cpg	866.54	J/mol×K	1157.26	Joback Method
cpg	868.70	J/mol×K	1193.84	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=U377739&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