Phthalic acid, di(2,4,5-trifluorobenzyl) ester

Inchi: InChI=1S/C22H12F6O4/c23-15-7-19(27)17(25)5-11(15)9-31-21(29)13-3-1-2-4-14(13)22(
InchiKey: XWTYXZKXXHJUFS-UHFFFAOYSA-N
Formula: C22H12F6O4
SMILES: O=C(OCc1cc(F)c(F)cc1F)c1ccccc1C(=O)OCc1cc(F)c(F)cc1F
Mol. weight [g/mol]: 454.32

Physical Properties

Property code	Value	Unit	Source
gf	-1232.52	kJ/mol	Joback Method
hf	-1534.37	kJ/mol	Joback Method
hfus	56.19	kJ/mol	Joback Method
hvap	89.44	kJ/mol	Joback Method
log10ws	-8.17		Crippen Method
logp	5.235		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
rinpol	2992.00		NIST Webbook
rinpol	2992.00		NIST Webbook
tb	965.86	K	Joback Method
tc	1187.70	K	Joback Method
tf	652.46	K	Joback Method
vc	1.099	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	826.46	J/mol×K	965.86	Joback Method
cpg	835.59	J/mol×K	1002.83	Joback Method
cpg	843.46	J/mol×K	1039.81	Joback Method
cpg	850.10	J/mol×K	1076.78	Joback Method
cpg	855.51	J/mol×K	1113.75	Joback Method
cpg	859.73	J/mol×K	1150.73	Joback Method
cpg	862.75	J/mol×K	1187.70	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=U415508&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