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

Inchi: InChI=1S/C22H22F4O4/c1-2-3-4-5-8-11-29-21(27)15-9-6-7-10-16(15)22(28)30-13-14-12

InchiKey: LIKBUXLLHRXIFU-UHFFFAOYSA-N

Formula: C22H22F4O4

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

Mol. weight [g/mol]: 426.40

Physical Properties

Property code	Value	Unit	Source
gf	-936.05	kJ/mol	Joback Method
hf	-1355.74	kJ/mol	Joback Method
hfus	56.77	kJ/mol	Joback Method
hvap	87.47	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	5.727		Crippen Method
mcvol	295.280	ml/mol	McGowan Method
pc	1247.73	kPa	Joback Method
rinpol	2511.00		NIST Webbook
rinpol	2511.00		NIST Webbook
tb	930.68	K	Joback Method
tc	1141.76	K	Joback Method
tf	599.82	K	Joback Method
vc	1.171	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	921.80	J/mol×K	930.68	Joback Method
cpg	934.38	J/mol×K	965.86	Joback Method
cpg	945.72	J/mol×K	1001.04	Joback Method
cpg	955.84	J/mol×K	1036.22	Joback Method
cpg	964.77	J/mol×K	1071.40	Joback Method
cpg	972.52	J/mol×K	1106.58	Joback Method
cpg	979.11	J/mol×K	1141.76	Joback Method

Sources

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=U377730&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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