Isophthalic acid, heptyl pentafluorobenzyl ester

Inchi: InChI=1S/C22H21F5O4/c1-2-3-4-5-6-10-30-21(28)13-8-7-9-14(11-13)22(29)31-12-15-16

InchiKey: KENQWTRUQXOWFH-UHFFFAOYSA-N

Formula: C22H21F5O4

SMILES: CCCCCCCOC(=O)c1cccc(C(=O)OCc2c(F)c(F)c(F)c(F)c2F)c1

Mol. weight [g/mol]: 444.39

Physical Properties

Property code	Value	Unit	Source
gf	-1140.49	kJ/mol	Joback Method
hf	-1563.32	kJ/mol	Joback Method
hfus	59.46	kJ/mol	Joback Method
hvap	87.32	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	5.866		Crippen Method
mcvol	297.050	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2701.00		NIST Webbook
rinpol	2701.00		NIST Webbook
tb	934.93	K	Joback Method
tc	1145.41	K	Joback Method
tf	612.93	K	Joback Method
vc	1.190	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	927.67	J/mol×K	934.93	Joback Method
cpg	939.93	J/mol×K	970.01	Joback Method
cpg	950.95	J/mol×K	1005.09	Joback Method
cpg	960.74	J/mol×K	1040.17	Joback Method
cpg	969.33	J/mol×K	1075.25	Joback Method
cpg	976.72	J/mol×K	1110.33	Joback Method
cpg	982.92	J/mol×K	1145.41	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=U344506&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