Terephthalic acid, hexyl 1-(pentafluorophenyl)ethyl ester

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

InchiKey: GISODLKDJKLMBH-UHFFFAOYSA-N

Formula: C22H21F5O4

SMILES: CCCCCCOC(=O)c1ccc(C(=O)OC(C)c2c(F)c(F)c(F)c(F)c2F)cc1

Mol. weight [g/mol]: 444.39

Physical Properties

Property code	Value	Unit	Source
gf	-1142.93	kJ/mol	Joback Method
hf	-1568.60	kJ/mol	Joback Method
hfus	55.93	kJ/mol	Joback Method
hvap	86.93	kJ/mol	Joback Method
log10ws	-8.20		Crippen Method
logp	6.037		Crippen Method
mcvol	297.050	ml/mol	McGowan Method
pc	1203.12	kPa	Joback Method
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
tb	934.49	K	Joback Method
tc	1145.43	K	Joback Method
tf	597.93	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.16	J/mol×K	934.49	Joback Method
cpg	940.40	J/mol×K	969.65	Joback Method
cpg	951.39	J/mol×K	1004.80	Joback Method
cpg	961.14	J/mol×K	1039.96	Joback Method
cpg	969.66	J/mol×K	1075.12	Joback Method
cpg	976.97	J/mol×K	1110.28	Joback Method
cpg	983.07	J/mol×K	1145.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416058&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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