Terephthalic acid, 1-(pentafluorophenyl)ethyl pentyl ester

Inchi: InChI=1S/C21H19F5O4/c1-3-4-5-10-29-20(27)12-6-8-13(9-7-12)21(28)30-11(2)14-15(22

InchiKey: SGZCYCBMTZJYNX-UHFFFAOYSA-N

Formula: C21H19F5O4

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

Mol. weight [g/mol]: 430.37

Physical Properties

Property code	Value	Unit	Source
gf	-1151.35	kJ/mol	Joback Method
hf	-1547.96	kJ/mol	Joback Method
hfus	53.34	kJ/mol	Joback Method
hvap	84.70	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	5.647		Crippen Method
mcvol	282.960	ml/mol	McGowan Method
pc	1287.44	kPa	Joback Method
rinpol	2550.00		NIST Webbook
rinpol	2550.00		NIST Webbook
tb	911.61	K	Joback Method
tc	1119.49	K	Joback Method
tf	586.66	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.01	J/mol×K	911.61	Joback Method
cpg	882.04	J/mol×K	946.26	Joback Method
cpg	892.89	J/mol×K	980.90	Joback Method
cpg	902.58	J/mol×K	1015.55	Joback Method
cpg	911.10	J/mol×K	1050.20	Joback Method
cpg	918.48	J/mol×K	1084.85	Joback Method
cpg	924.72	J/mol×K	1119.49	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416057&Units=SI

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