Terephthalic acid, isobutyl 1-(pentafluorophenyl)ethyl ester

Inchi: InChI=1S/C20H17F5O4/c1-9(2)8-28-19(26)11-4-6-12(7-5-11)20(27)29-10(3)13-14(21)16

InchiKey: NTAVHZFZIWRNBX-UHFFFAOYSA-N

Formula: C20H17F5O4

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

Mol. weight [g/mol]: 416.34

Physical Properties

Property code	Value	Unit	Source
gf	-1162.21	kJ/mol	Joback Method
hf	-1532.60	kJ/mol	Joback Method
hfus	47.23	kJ/mol	Joback Method
hvap	82.09	kJ/mol	Joback Method
log10ws	-7.12		Crippen Method
logp	5.113		Crippen Method
mcvol	268.870	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	2348.00		NIST Webbook
rinpol	2348.00		NIST Webbook
tb	888.29	K	Joback Method
tc	1095.30	K	Joback Method
tf	560.39	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.05	J/mol×K	888.29	Joback Method
cpg	824.90	J/mol×K	922.79	Joback Method
cpg	835.62	J/mol×K	957.29	Joback Method
cpg	845.21	J/mol×K	991.80	Joback Method
cpg	853.67	J/mol×K	1026.30	Joback Method
cpg	861.03	J/mol×K	1060.80	Joback Method
cpg	867.27	J/mol×K	1095.30	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=U416055&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