Isophthalic acid, pentafluorobenzyl propyl ester

Inchi: InChI=1S/C18H13F5O4/c1-2-6-26-17(24)9-4-3-5-10(7-9)18(25)27-8-11-12(19)14(21)16(2

InchiKey: PULGSEYGQJVUDH-UHFFFAOYSA-N

Formula: C18H13F5O4

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

Mol. weight [g/mol]: 388.29

Physical Properties

Property code	Value	Unit	Source
gf	-1174.17	kJ/mol	Joback Method
hf	-1480.76	kJ/mol	Joback Method
hfus	49.10	kJ/mol	Joback Method
hvap	78.41	kJ/mol	Joback Method
log10ws	-6.56		Crippen Method
logp	4.306		Crippen Method
mcvol	240.690	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinpol	2284.00		NIST Webbook
rinpol	2284.00		NIST Webbook
tb	843.41	K	Joback Method
tc	1045.21	K	Joback Method
tf	567.85	K	Joback Method
vc	0.966	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.14	J/mol×K	843.41	Joback Method
cpg	710.33	J/mol×K	877.04	Joback Method
cpg	720.56	J/mol×K	910.68	Joback Method
cpg	729.83	J/mol×K	944.31	Joback Method
cpg	738.14	J/mol×K	977.95	Joback Method
cpg	745.48	J/mol×K	1011.58	Joback Method
cpg	751.88	J/mol×K	1045.21	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=U344503&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