Phthalic acid, isobutyl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C19H16F4O4/c1-10(2)8-26-18(24)12-5-3-4-6-13(12)19(25)27-9-11-7-14(20)16

InchiKey: JXTOTORXXQWOPP-UHFFFAOYSA-N

Formula: C19H16F4O4

SMILES: CC(C)COC(=O)c1ccccc1C(=O)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 384.32

Physical Properties

Property code	Value	Unit	Source
gf	-963.75	kJ/mol	Joback Method
hf	-1299.10	kJ/mol	Joback Method
hfus	45.47	kJ/mol	Joback Method
hvap	80.41	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	4.413		Crippen Method
mcvol	253.010	ml/mol	McGowan Method
pc	1556.12	kPa	Joback Method
rinpol	2166.00		NIST Webbook
rinpol	2166.00		NIST Webbook
tb	861.60	K	Joback Method
tc	1069.27	K	Joback Method
tf	551.01	K	Joback Method
vc	0.998	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	749.67	J/mol×K	861.60	Joback Method
cpg	761.65	J/mol×K	896.21	Joback Method
cpg	772.56	J/mol×K	930.82	Joback Method
cpg	782.40	J/mol×K	965.44	Joback Method
cpg	791.17	J/mol×K	1000.05	Joback Method
cpg	798.90	J/mol×K	1034.66	Joback Method
cpg	805.57	J/mol×K	1069.27	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=U377726&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