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

Inchi: InChI=1S/C18H14F4O4/c1-2-7-25-17(23)11-5-3-4-6-12(11)18(24)26-9-10-8-13(19)15(21

InchiKey: ZPNJQMGSFIVIHJ-UHFFFAOYSA-N

Formula: C18H14F4O4

SMILES: CCCOC(=O)c1ccccc1C(=O)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 370.30

Physical Properties

Property code	Value	Unit	Source
gf	-969.73	kJ/mol	Joback Method
hf	-1273.18	kJ/mol	Joback Method
hfus	46.41	kJ/mol	Joback Method
hvap	78.57	kJ/mol	Joback Method
log10ws	-6.23		Crippen Method
logp	4.167		Crippen Method
mcvol	238.920	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	2105.00		NIST Webbook
tb	839.16	K	Joback Method
tc	1044.76	K	Joback Method
tf	554.74	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	693.04	J/mol×K	839.16	Joback Method
cpg	704.68	J/mol×K	873.43	Joback Method
cpg	715.31	J/mol×K	907.69	Joback Method
cpg	724.95	J/mol×K	941.96	Joback Method
cpg	733.61	J/mol×K	976.22	Joback Method
cpg	741.28	J/mol×K	1010.49	Joback Method
cpg	747.98	J/mol×K	1044.76	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=U377725&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