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

Inchi: InChI=1S/C17H12F4O4/c1-2-24-16(22)10-5-3-4-6-11(10)17(23)25-8-9-7-12(18)14(20)15

InchiKey: XPDHEHOKFQQNRZ-UHFFFAOYSA-N

Formula: C17H12F4O4

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

Mol. weight [g/mol]: 356.27

Physical Properties

Property code	Value	Unit	Source
gf	-978.15	kJ/mol	Joback Method
hf	-1252.54	kJ/mol	Joback Method
hfus	43.82	kJ/mol	Joback Method
hvap	76.34	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	3.777		Crippen Method
mcvol	224.830	ml/mol	McGowan Method
pc	1809.23	kPa	Joback Method
rinpol	2014.00		NIST Webbook
rinpol	2014.00		NIST Webbook
tb	816.28	K	Joback Method
tc	1022.34	K	Joback Method
tf	543.47	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	637.85	J/mol×K	816.28	Joback Method
cpg	649.18	J/mol×K	850.62	Joback Method
cpg	659.56	J/mol×K	884.97	Joback Method
cpg	668.99	J/mol×K	919.31	Joback Method
cpg	677.48	J/mol×K	953.65	Joback Method
cpg	685.03	J/mol×K	987.99	Joback Method
cpg	691.63	J/mol×K	1022.34	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377724&Units=SI
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

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