Phthalic acid, pentafluorophenyl propyl ester

Inchi: InChI=1S/C17H11F5O4/c1-2-7-25-16(23)8-5-3-4-6-9(8)17(24)26-15-13(21)11(19)10(18)
InchiKey: DZCVRGBFEARGDE-UHFFFAOYSA-N
Formula: C17H11F5O4
SMILES: CCCOC(=O)c1ccccc1C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 374.26

Physical Properties

Property code	Value	Unit	Source
gf	-1182.59	kJ/mol	Joback Method
hf	-1460.12	kJ/mol	Joback Method
hfus	46.51	kJ/mol	Joback Method
hvap	76.19	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	4.168		Crippen Method
mcvol	226.600	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	1980.00		NIST Webbook
rinpol	1980.00		NIST Webbook
tb	820.53	K	Joback Method
tc	1022.07	K	Joback Method
tf	556.58	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	643.99	J/mol×K	820.53	Joback Method
cpg	654.85	J/mol×K	854.12	Joback Method
cpg	664.80	J/mol×K	887.71	Joback Method
cpg	673.85	J/mol×K	921.30	Joback Method
cpg	681.98	J/mol×K	954.89	Joback Method
cpg	689.20	J/mol×K	988.48	Joback Method
cpg	695.52	J/mol×K	1022.07	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=U356189&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