Phthalic acid, ethyl pentafluorophenyl ester

Inchi: InChI=1S/C16H9F5O4/c1-2-24-15(22)7-5-3-4-6-8(7)16(23)25-14-12(20)10(18)9(17)11(19)13(14)21

InchiKey: WKLCYLCSZYYOJG-UHFFFAOYSA-N

Formula: C16H9F5O4

SMILES: CCOC(=O)c1ccccc1C(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 360.23

Physical Properties

Property code	Value	Unit	Source
gf	-1191.01	kJ/mol	Joback Method
hf	-1439.48	kJ/mol	Joback Method
hfus	43.92	kJ/mol	Joback Method
hvap	73.96	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	3.778		Crippen Method
mcvol	212.510	ml/mol	McGowan Method
pc	1865.94	kPa	Joback Method
rinpol	1898.00		NIST Webbook
tb	797.65	K	Joback Method
tc	999.58	K	Joback Method
tf	545.31	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	589.78	J/mol×K	797.65	Joback Method
cpg	600.27	J/mol×K	831.31	Joback Method
cpg	609.90	J/mol×K	864.96	Joback Method
cpg	618.67	J/mol×K	898.62	Joback Method
cpg	626.58	J/mol×K	932.27	Joback Method
cpg	633.63	J/mol×K	965.93	Joback Method
cpg	639.81	J/mol×K	999.58	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=U356188&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