Terephthalic acid, 1-(pentafluorophenyl)ethyl propyl ester

Inchi: InChI=1S/C19H15F5O4/c1-3-8-27-18(25)10-4-6-11(7-5-10)19(26)28-9(2)12-13(20)15(22
InchiKey: BYFZRFAAFJWWND-UHFFFAOYSA-N
Formula: C19H15F5O4
SMILES: CCCOC(=O)c1ccc(C(=O)OC(C)c2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]: 402.31

Physical Properties

Property code	Value	Unit	Source
gf	-1168.19	kJ/mol	Joback Method
hf	-1506.68	kJ/mol	Joback Method
hfus	48.16	kJ/mol	Joback Method
hvap	80.25	kJ/mol	Joback Method
log10ws	-6.94		Crippen Method
logp	4.867		Crippen Method
mcvol	254.780	ml/mol	McGowan Method
pc	1485.00	kPa	Joback Method
rinpol	2298.00		NIST Webbook
rinpol	2298.00		NIST Webbook
tb	865.85	K	Joback Method
tc	1070.14	K	Joback Method
tf	564.12	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	755.72	J/mol×K	865.85	Joback Method
cpg	767.28	J/mol×K	899.90	Joback Method
cpg	777.78	J/mol×K	933.95	Joback Method
cpg	787.25	J/mol×K	968.00	Joback Method
cpg	795.67	J/mol×K	1002.05	Joback Method
cpg	803.06	J/mol×K	1036.09	Joback Method
cpg	809.41	J/mol×K	1070.14	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=U416054&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