Phthalic acid, hexadecyl pentafluorophenyl ester

Inchi: InChI=1S/C30H37F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-38-29(36)21-18-15-16

InchiKey: BDAUSKWXXIZRCB-UHFFFAOYSA-N

Formula: C30H37F5O4

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

Mol. weight [g/mol]: 556.60

Physical Properties

Property code	Value	Unit	Source
gf	-1073.13	kJ/mol	Joback Method
hf	-1728.44	kJ/mol	Joback Method
hfus	80.18	kJ/mol	Joback Method
hvap	105.12	kJ/mol	Joback Method
log10ws	-11.74		Crippen Method
logp	9.239		Crippen Method
mcvol	409.770	ml/mol	McGowan Method
pc	746.92	kPa	Joback Method
rinpol	3258.00		NIST Webbook
rinpol	3258.00		NIST Webbook
tb	1117.97	K	Joback Method
tc	1396.46	K	Joback Method
tf	703.09	K	Joback Method
vc	1.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1409.64	J/mol×K	1117.97	Joback Method
cpg	1423.69	J/mol×K	1164.38	Joback Method
cpg	1435.27	J/mol×K	1210.80	Joback Method
cpg	1444.47	J/mol×K	1257.21	Joback Method
cpg	1451.36	J/mol×K	1303.63	Joback Method
cpg	1456.04	J/mol×K	1350.04	Joback Method
cpg	1458.59	J/mol×K	1396.46	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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