Phthalic acid, heptadecyl pentafluorophenyl ester

Inchi: InChI=1S/C31H39F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-39-30(37)22-19-16

InchiKey: VGINDGOSKODBBO-UHFFFAOYSA-N

Formula: C31H39F5O4

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

Mol. weight [g/mol]: 570.63

Physical Properties

Property code	Value	Unit	Source
gf	-1064.71	kJ/mol	Joback Method
hf	-1749.08	kJ/mol	Joback Method
hfus	82.77	kJ/mol	Joback Method
hvap	107.35	kJ/mol	Joback Method
log10ws	-12.16		Crippen Method
logp	9.630		Crippen Method
mcvol	423.860	ml/mol	McGowan Method
pc	709.22	kPa	Joback Method
rinpol	3365.00		NIST Webbook
tb	1140.85	K	Joback Method
tc	1434.31	K	Joback Method
tf	714.36	K	Joback Method
vc	1.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1471.22	J/mol×K	1140.85	Joback Method
cpg	1485.48	J/mol×K	1189.76	Joback Method
cpg	1496.99	J/mol×K	1238.67	Joback Method
cpg	1505.85	J/mol×K	1287.58	Joback Method
cpg	1512.19	J/mol×K	1336.49	Joback Method
cpg	1516.11	J/mol×K	1385.40	Joback Method
cpg	1517.72	J/mol×K	1434.31	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=U356366&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

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