Phthalic acid, octadecyl pentafluorophenyl ester

Inchi: InChI=1S/C32H41F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-19-22-40-31(38)23-20

InchiKey: FAACVQBWPICRQZ-UHFFFAOYSA-N

Formula: C32H41F5O4

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

Mol. weight [g/mol]: 584.66

Physical Properties

Property code	Value	Unit	Source
gf	-1056.29	kJ/mol	Joback Method
hf	-1769.72	kJ/mol	Joback Method
hfus	85.36	kJ/mol	Joback Method
hvap	109.58	kJ/mol	Joback Method
log10ws	-12.58		Crippen Method
logp	10.020		Crippen Method
mcvol	437.950	ml/mol	McGowan Method
pc	674.30	kPa	Joback Method
rinpol	3474.00		NIST Webbook
tb	1163.73	K	Joback Method
tc	1473.98	K	Joback Method
tf	725.63	K	Joback Method
vc	1.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1532.97	J/mol×K	1163.73	Joback Method
cpg	1547.42	J/mol×K	1215.44	Joback Method
cpg	1558.80	J/mol×K	1267.15	Joback Method
cpg	1567.25	J/mol×K	1318.86	Joback Method
cpg	1572.91	J/mol×K	1370.56	Joback Method
cpg	1575.93	J/mol×K	1422.27	Joback Method
cpg	1576.45	J/mol×K	1473.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356385&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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