Phthalic acid, hexadecyl 2,3,4,5-tetrafluorobenzyl ester

Inchi: InChI=1S/C31H40F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-17-20-38-30(36)24-18-15-16

InchiKey: LUZPEAQLJSNLOO-UHFFFAOYSA-N

Formula: C31H40F4O4

SMILES: CCCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)c(F)c(F)c1F

Mol. weight [g/mol]: 552.64

Physical Properties

Property code	Value	Unit	Source
gf	-860.27	kJ/mol	Joback Method
hf	-1541.50	kJ/mol	Joback Method
hfus	80.08	kJ/mol	Joback Method
hvap	107.51	kJ/mol	Joback Method
log10ws	-11.67		Crippen Method
logp	9.238		Crippen Method
mcvol	422.090	ml/mol	McGowan Method
pc	732.44	kPa	Joback Method
rinpol	3329.00		NIST Webbook
rinpol	3329.00		NIST Webbook
tb	1136.60	K	Joback Method
tc	1420.50	K	Joback Method
tf	701.25	K	Joback Method
vc	1.675	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1466.59	J/mol×K	1136.60	Joback Method
cpg	1481.05	J/mol×K	1183.92	Joback Method
cpg	1493.01	J/mol×K	1231.23	Joback Method
cpg	1502.57	J/mol×K	1278.55	Joback Method
cpg	1509.84	J/mol×K	1325.87	Joback Method
cpg	1514.95	J/mol×K	1373.19	Joback Method
cpg	1518.00	J/mol×K	1420.50	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=U377738&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