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

Inchi: InChI=1S/C30H38F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-19-37-29(35)23-17-14-15-18

InchiKey: UFYLVOLVGISCIO-UHFFFAOYSA-N

Formula: C30H38F4O4

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

Mol. weight [g/mol]: 538.61

Physical Properties

Property code	Value	Unit	Source
gf	-868.69	kJ/mol	Joback Method
hf	-1520.86	kJ/mol	Joback Method
hfus	77.49	kJ/mol	Joback Method
hvap	105.28	kJ/mol	Joback Method
log10ws	-11.25		Crippen Method
logp	8.848		Crippen Method
mcvol	408.000	ml/mol	McGowan Method
pc	772.03	kPa	Joback Method
rinpol	3228.00		NIST Webbook
tb	1113.72	K	Joback Method
tc	1384.08	K	Joback Method
tf	689.98	K	Joback Method
vc	1.619	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1404.81	J/mol×K	1113.72	Joback Method
cpg	1419.05	J/mol×K	1158.78	Joback Method
cpg	1431.01	J/mol×K	1203.84	Joback Method
cpg	1440.78	J/mol×K	1248.90	Joback Method
cpg	1448.47	J/mol×K	1293.96	Joback Method
cpg	1454.14	J/mol×K	1339.02	Joback Method
cpg	1457.91	J/mol×K	1384.08	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=U377737&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