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

Inchi: InChI=1S/C25H28F4O4/c1-2-3-4-5-6-7-8-11-14-32-24(30)18-12-9-10-13-19(18)25(31)33

InchiKey: PNGFSNAOGROERM-UHFFFAOYSA-N

Formula: C25H28F4O4

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

Mol. weight [g/mol]: 468.48

Physical Properties

Property code	Value	Unit	Source
gf	-910.79	kJ/mol	Joback Method
hf	-1417.66	kJ/mol	Joback Method
hfus	64.54	kJ/mol	Joback Method
hvap	94.15	kJ/mol	Joback Method
log10ws	-9.16		Crippen Method
logp	6.897		Crippen Method
mcvol	337.550	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	2826.00		NIST Webbook
tb	999.32	K	Joback Method
tc	1223.82	K	Joback Method
tf	633.63	K	Joback Method
vc	1.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1099.92	J/mol×K	999.32	Joback Method
cpg	1113.09	J/mol×K	1036.74	Joback Method
cpg	1124.77	J/mol×K	1074.15	Joback Method
cpg	1134.98	J/mol×K	1111.57	Joback Method
cpg	1143.76	J/mol×K	1148.98	Joback Method
cpg	1151.14	J/mol×K	1186.40	Joback Method
cpg	1157.16	J/mol×K	1223.82	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=U377733&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