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

Inchi: InChI=1S/C28H34F4O4/c1-2-3-4-5-6-7-8-9-10-11-14-17-35-27(33)21-15-12-13-16-22(21

InchiKey: FFKRZVYPLGPNQJ-UHFFFAOYSA-N

Formula: C28H34F4O4

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

Mol. weight [g/mol]: 510.56

Physical Properties

Property code	Value	Unit	Source
gf	-885.53	kJ/mol	Joback Method
hf	-1479.58	kJ/mol	Joback Method
hfus	72.31	kJ/mol	Joback Method
hvap	100.83	kJ/mol	Joback Method
log10ws	-10.42		Crippen Method
logp	8.068		Crippen Method
mcvol	379.820	ml/mol	McGowan Method
pc	861.50	kPa	Joback Method
rinpol	3126.00		NIST Webbook
tb	1067.96	K	Joback Method
tc	1315.93	K	Joback Method
tf	667.44	K	Joback Method
vc	1.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1281.93	J/mol×K	1067.96	Joback Method
cpg	1295.73	J/mol×K	1109.29	Joback Method
cpg	1307.63	J/mol×K	1150.62	Joback Method
cpg	1317.69	J/mol×K	1191.94	Joback Method
cpg	1325.97	J/mol×K	1233.27	Joback Method
cpg	1332.53	J/mol×K	1274.60	Joback Method
cpg	1337.44	J/mol×K	1315.93	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=U377736&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