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

Inchi: InChI=1S/C21H20F4O4/c1-2-3-4-7-10-28-20(26)14-8-5-6-9-15(14)21(27)29-12-13-11-16
InchiKey: BOPCDMJUVHYXRB-UHFFFAOYSA-N
Formula: C21H20F4O4
SMILES: CCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]: 412.37

Physical Properties

Property code	Value	Unit	Source
gf	-944.47	kJ/mol	Joback Method
hf	-1335.10	kJ/mol	Joback Method
hfus	54.18	kJ/mol	Joback Method
hvap	85.25	kJ/mol	Joback Method
log10ws	-7.49		Crippen Method
logp	5.337		Crippen Method
mcvol	281.190	ml/mol	McGowan Method
pc	1336.86	kPa	Joback Method
rinpol	2406.00		NIST Webbook
rinpol	2406.00		NIST Webbook
tb	907.80	K	Joback Method
tc	1116.31	K	Joback Method
tf	588.55	K	Joback Method
vc	1.115	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	863.55	J/mol×K	907.80	Joback Method
cpg	875.92	J/mol×K	942.55	Joback Method
cpg	887.11	J/mol×K	977.30	Joback Method
cpg	897.16	J/mol×K	1012.05	Joback Method
cpg	906.07	J/mol×K	1046.80	Joback Method
cpg	913.87	J/mol×K	1081.55	Joback Method
cpg	920.55	J/mol×K	1116.31	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377729&Units=SI

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