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

Inchi: InChI=1S/C23H24F4O4/c1-2-3-4-5-6-9-12-30-22(28)16-10-7-8-11-17(16)23(29)31-14-15
InchiKey: NVRVALZMIOYJLQ-UHFFFAOYSA-N
Formula: C23H24F4O4
SMILES: CCCCCCCCOC(=O)c1ccccc1C(=O)OCc1cc(F)c(F)c(F)c1F
Mol. weight [g/mol]: 440.43

Physical Properties

Property code	Value	Unit	Source
gf	-927.63	kJ/mol	Joback Method
hf	-1376.38	kJ/mol	Joback Method
hfus	59.36	kJ/mol	Joback Method
hvap	89.70	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	6.117		Crippen Method
mcvol	309.370	ml/mol	McGowan Method
pc	1167.22	kPa	Joback Method
rinpol	2618.00		NIST Webbook
rinpol	2618.00		NIST Webbook
tb	953.56	K	Joback Method
tc	1168.12	K	Joback Method
tf	611.09	K	Joback Method
vc	1.228	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.65	J/mol×K	953.56	Joback Method
cpg	993.43	J/mol×K	989.32	Joback Method
cpg	1004.89	J/mol×K	1025.08	Joback Method
cpg	1015.07	J/mol×K	1060.84	Joback Method
cpg	1023.98	J/mol×K	1096.60	Joback Method
cpg	1031.65	J/mol×K	1132.36	Joback Method
cpg	1038.10	J/mol×K	1168.12	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=U377731&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