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

Inchi: InChI=1S/C24H26F4O4/c1-2-3-4-5-6-7-10-13-31-23(29)17-11-8-9-12-18(17)24(30)32-15

InchiKey: VCUNYTDIQNOZCX-UHFFFAOYSA-N

Formula: C24H26F4O4

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

Mol. weight [g/mol]: 454.45

Physical Properties

Property code	Value	Unit	Source
gf	-919.21	kJ/mol	Joback Method
hf	-1397.02	kJ/mol	Joback Method
hfus	61.95	kJ/mol	Joback Method
hvap	91.92	kJ/mol	Joback Method
log10ws	-8.74		Crippen Method
logp	6.507		Crippen Method
mcvol	323.460	ml/mol	McGowan Method
pc	1094.27	kPa	Joback Method
rinpol	2726.00		NIST Webbook
tb	976.44	K	Joback Method
tc	1195.45	K	Joback Method
tf	622.36	K	Joback Method
vc	1.284	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1040.04	J/mol×K	976.44	Joback Method
cpg	1053.02	J/mol×K	1012.94	Joback Method
cpg	1064.59	J/mol×K	1049.44	Joback Method
cpg	1074.80	J/mol×K	1085.95	Joback Method
cpg	1083.66	J/mol×K	1122.45	Joback Method
cpg	1091.21	J/mol×K	1158.95	Joback Method
cpg	1097.47	J/mol×K	1195.45	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=U377732&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