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

Inchi: InChI=1S/C20H18F4O4/c1-2-3-6-9-27-19(25)13-7-4-5-8-14(13)20(26)28-11-12-10-15(21

InchiKey: XRBULHLKHFVCRE-UHFFFAOYSA-N

Formula: C20H18F4O4

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

Mol. weight [g/mol]: 398.35

Physical Properties

Property code	Value	Unit	Source
gf	-952.89	kJ/mol	Joback Method
hf	-1314.46	kJ/mol	Joback Method
hfus	51.59	kJ/mol	Joback Method
hvap	83.02	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	4.947		Crippen Method
mcvol	267.100	ml/mol	McGowan Method
pc	1435.89	kPa	Joback Method
rinpol	2309.00		NIST Webbook
tb	884.92	K	Joback Method
tc	1091.69	K	Joback Method
tf	577.28	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	805.96	J/mol×K	884.92	Joback Method
cpg	818.11	J/mol×K	919.38	Joback Method
cpg	829.14	J/mol×K	953.84	Joback Method
cpg	839.09	J/mol×K	988.30	Joback Method
cpg	847.95	J/mol×K	1022.77	Joback Method
cpg	855.74	J/mol×K	1057.23	Joback Method
cpg	862.48	J/mol×K	1091.69	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377728&Units=SI
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

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