Phthalic acid, 2,2,3,3,4,4,4-heptafluorobutyl pentyl ester

Inchi: InChI=1S/C17H17F7O4/c1-2-3-6-9-27-13(25)11-7-4-5-8-12(11)14(26)28-10-15(18,19)16

InchiKey: MOJADYZTEIBFCJ-UHFFFAOYSA-N

Formula: C17H17F7O4

SMILES: CCCCCOC(=O)c1ccccc1C(=O)OCC(F)(F)C(F)(F)C(F)(F)F

Mol. weight [g/mol]: 418.30

Physical Properties

Property code	Value	Unit	Source
gf	-1627.95	kJ/mol	Joback Method
hf	-2057.77	kJ/mol	Joback Method
hfus	38.33	kJ/mol	Joback Method
hvap	65.08	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.023		Crippen Method
mcvol	253.900	ml/mol	McGowan Method
pc	1371.74	kPa	Joback Method
rinpol	1842.00		NIST Webbook
rinpol	1842.00		NIST Webbook
tb	757.80	K	Joback Method
tc	940.48	K	Joback Method
tf	476.00	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	764.02	J/mol×K	757.80	Joback Method
cpg	776.77	J/mol×K	788.25	Joback Method
cpg	788.63	J/mol×K	818.69	Joback Method
cpg	799.66	J/mol×K	849.14	Joback Method
cpg	809.90	J/mol×K	879.59	Joback Method
cpg	819.40	J/mol×K	910.03	Joback Method
cpg	828.23	J/mol×K	940.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415543&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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