Isophthalic acid, 2,2,3,3,4,4,5,5-octafluoropentyl octyl ester

Inchi: InChI=1S/C21H24F8O4/c1-2-3-4-5-6-7-11-32-16(30)14-9-8-10-15(12-14)17(31)33-13-19
InchiKey: ZQQLWTYGYZUACA-UHFFFAOYSA-N
Formula: C21H24F8O4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1
Mol. weight [g/mol]: 492.40

Physical Properties

Property code	Value	Unit	Source
gf	-1791.52	kJ/mol	Joback Method
hf	-2341.72	kJ/mol	Joback Method
hfus	48.25	kJ/mol	Joback Method
hvap	72.78	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	6.532		Crippen Method
mcvol	312.030	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
rinpol	2291.00		NIST Webbook
rinpol	2291.00		NIST Webbook
tb	848.15	K	Joback Method
tc	1038.93	K	Joback Method
tf	506.67	K	Joback Method
vc	1.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	998.92	J/mol×K	848.15	Joback Method
cpg	1012.98	J/mol×K	879.95	Joback Method
cpg	1026.05	J/mol×K	911.74	Joback Method
cpg	1038.20	J/mol×K	943.54	Joback Method
cpg	1049.50	J/mol×K	975.34	Joback Method
cpg	1060.01	J/mol×K	1007.13	Joback Method
cpg	1069.82	J/mol×K	1038.93	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=U356592&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