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

Inchi: InChI=1S/C22H26F8O4/c1-2-3-4-5-6-7-8-12-33-17(31)15-10-9-11-16(13-15)18(32)34-14

InchiKey: RNZHXANXFNXXPN-UHFFFAOYSA-N

Formula: C22H26F8O4

SMILES: CCCCCCCCCOC(=O)c1cccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1

Mol. weight [g/mol]: 506.43

Physical Properties

Property code	Value	Unit	Source
gf	-1783.10	kJ/mol	Joback Method
hf	-2362.36	kJ/mol	Joback Method
hfus	50.84	kJ/mol	Joback Method
hvap	75.00	kJ/mol	Joback Method
log10ws	-8.24		Crippen Method
logp	6.922		Crippen Method
mcvol	326.120	ml/mol	McGowan Method
pc	966.27	kPa	Joback Method
rinpol	2382.00		NIST Webbook
tb	871.03	K	Joback Method
tc	1066.39	K	Joback Method
tf	517.94	K	Joback Method
vc	1.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1057.57	J/mol×K	871.03	Joback Method
cpg	1072.09	J/mol×K	903.59	Joback Method
cpg	1085.57	J/mol×K	936.15	Joback Method
cpg	1098.10	J/mol×K	968.71	Joback Method
cpg	1109.75	J/mol×K	1001.27	Joback Method
cpg	1120.60	J/mol×K	1033.83	Joback Method
cpg	1130.74	J/mol×K	1066.39	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356593&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