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

Inchi: InChI=1S/C20H22F8O4/c1-2-3-4-5-6-10-31-15(29)13-8-7-9-14(11-13)16(30)32-12-18(23

InchiKey: ZKMSQZNUIRRCFL-UHFFFAOYSA-N

Formula: C20H22F8O4

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

Mol. weight [g/mol]: 478.37

Physical Properties

Property code	Value	Unit	Source
gf	-1799.94	kJ/mol	Joback Method
hf	-2321.08	kJ/mol	Joback Method
hfus	45.66	kJ/mol	Joback Method
hvap	70.55	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.142		Crippen Method
mcvol	297.940	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	2191.00		NIST Webbook
rinpol	2191.00		NIST Webbook
tb	825.27	K	Joback Method
tc	1012.33	K	Joback Method
tf	495.40	K	Joback Method
vc	1.200	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	941.01	J/mol×K	825.27	Joback Method
cpg	954.66	J/mol×K	856.45	Joback Method
cpg	967.35	J/mol×K	887.62	Joback Method
cpg	979.14	J/mol×K	918.80	Joback Method
cpg	990.11	J/mol×K	949.97	Joback Method
cpg	1000.30	J/mol×K	981.15	Joback Method
cpg	1009.80	J/mol×K	1012.33	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356591&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