Terephthalic acid, 2,2,3,4,4,4-hexafluorobutyl undecyl ester

Inchi: InChI=1S/C23H30F6O4/c1-2-3-4-5-6-7-8-9-10-15-32-19(30)17-11-13-18(14-12-17)20(31

InchiKey: GITHLSUDMPWXIN-UHFFFAOYSA-N

Formula: C23H30F6O4

SMILES: CCCCCCCCCCCOC(=O)c1ccc(C(=O)OCC(F)(F)C(F)C(F)(F)F)cc1

Mol. weight [g/mol]: 484.47

Physical Properties

Property code	Value	Unit	Source
gf	-1387.90	kJ/mol	Joback Method
hf	-1982.03	kJ/mol	Joback Method
hfus	54.68	kJ/mol	Joback Method
hvap	80.16	kJ/mol	Joback Method
log10ws	-8.34		Crippen Method
logp	7.067		Crippen Method
mcvol	336.670	ml/mol	McGowan Method
pc	951.42	kPa	Joback Method
rinpol	1648.00		NIST Webbook
rinpol	1648.00		NIST Webbook
tb	898.60	K	Joback Method
tc	1100.20	K	Joback Method
tf	525.61	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1102.05	J/mol×K	898.60	Joback Method
cpg	1117.50	J/mol×K	932.20	Joback Method
cpg	1131.82	J/mol×K	965.80	Joback Method
cpg	1145.06	J/mol×K	999.40	Joback Method
cpg	1157.32	J/mol×K	1033.00	Joback Method
cpg	1168.64	J/mol×K	1066.60	Joback Method
cpg	1179.12	J/mol×K	1100.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415758&Units=SI

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