Terephthalic acid, 2,2,3,3,3-pentafluoropropyl undecyl ester

Inchi: InChI=1S/C22H29F5O4/c1-2-3-4-5-6-7-8-9-10-15-30-19(28)17-11-13-18(14-12-17)20(29

InchiKey: JLIOXZXJZQFDKT-UHFFFAOYSA-N

Formula: C22H29F5O4

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

Mol. weight [g/mol]: 452.46

Physical Properties

Property code	Value	Unit	Source
gf	-1199.07	kJ/mol	Joback Method
hf	-1760.00	kJ/mol	Joback Method
hfus	52.53	kJ/mol	Joback Method
hvap	79.14	kJ/mol	Joback Method
log10ws	-7.96		Crippen Method
logp	6.729		Crippen Method
mcvol	320.810	ml/mol	McGowan Method
pc	1034.57	kPa	Joback Method
rinpol	2472.00		NIST Webbook
rinpol	2472.00		NIST Webbook
tb	876.89	K	Joback Method
tc	1074.12	K	Joback Method
tf	528.75	K	Joback Method
vc	1.276	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1034.54	J/mol×K	876.89	Joback Method
cpg	1049.73	J/mol×K	909.76	Joback Method
cpg	1063.85	J/mol×K	942.63	Joback Method
cpg	1076.95	J/mol×K	975.50	Joback Method
cpg	1089.10	J/mol×K	1008.37	Joback Method
cpg	1100.37	J/mol×K	1041.25	Joback Method
cpg	1110.81	J/mol×K	1074.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415782&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