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

Inchi: InChI=1S/C28H38F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-18-39-23(37)21-16-15-17-22
InchiKey: JADKPCRIFLKOAJ-UHFFFAOYSA-N
Formula: C28H38F8O4
SMILES: CCCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1
Mol. weight [g/mol]: 590.59

Physical Properties

Property code	Value	Unit	Source
gf	-1732.58	kJ/mol	Joback Method
hf	-2486.20	kJ/mol	Joback Method
hfus	66.38	kJ/mol	Joback Method
hvap	88.36	kJ/mol	Joback Method
log10ws	-10.75		Crippen Method
logp	9.262		Crippen Method
mcvol	410.660	ml/mol	McGowan Method
pc	695.08	kPa	Joback Method
rinpol	2960.00		NIST Webbook
tb	1008.31	K	Joback Method
tc	1253.50	K	Joback Method
tf	585.56	K	Joback Method
vc	1.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1422.79	J/mol×K	1008.31	Joback Method
cpg	1441.21	J/mol×K	1049.17	Joback Method
cpg	1458.22	J/mol×K	1090.04	Joback Method
cpg	1474.01	J/mol×K	1130.90	Joback Method
cpg	1488.76	J/mol×K	1171.77	Joback Method
cpg	1502.66	J/mol×K	1212.63	Joback Method
cpg	1515.89	J/mol×K	1253.50	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=U356599&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