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

Inchi: InChI=1S/C26H34F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-37-21(35)19-14-13-15-20(17-19

InchiKey: CUHIGUXYNMCZLF-UHFFFAOYSA-N

Formula: C26H34F8O4

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

Mol. weight [g/mol]: 562.53

Physical Properties

Property code	Value	Unit	Source
gf	-1749.42	kJ/mol	Joback Method
hf	-2444.92	kJ/mol	Joback Method
hfus	61.20	kJ/mol	Joback Method
hvap	83.91	kJ/mol	Joback Method
log10ws	-9.91		Crippen Method
logp	8.482		Crippen Method
mcvol	382.480	ml/mol	McGowan Method
pc	771.18	kPa	Joback Method
rinpol	2758.00		NIST Webbook
rinpol	2758.00		NIST Webbook
tb	962.55	K	Joback Method
tc	1186.30	K	Joback Method
tf	563.02	K	Joback Method
vc	1.536	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1298.77	J/mol×K	962.55	Joback Method
cpg	1315.60	J/mol×K	999.84	Joback Method
cpg	1331.18	J/mol×K	1037.13	Joback Method
cpg	1345.63	J/mol×K	1074.42	Joback Method
cpg	1359.09	J/mol×K	1111.72	Joback Method
cpg	1371.70	J/mol×K	1149.01	Joback Method
cpg	1383.59	J/mol×K	1186.30	Joback Method

Sources

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=U356597&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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