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

Inchi: InChI=1S/C25H32F8O4/c1-2-3-4-5-6-7-8-9-10-11-15-36-20(34)18-13-12-14-19(16-18)21

InchiKey: KZDIOFVHNZAQPK-UHFFFAOYSA-N

Formula: C25H32F8O4

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

Mol. weight [g/mol]: 548.51

Physical Properties

Property code	Value	Unit	Source
gf	-1757.84	kJ/mol	Joback Method
hf	-2424.28	kJ/mol	Joback Method
hfus	58.61	kJ/mol	Joback Method
hvap	81.68	kJ/mol	Joback Method
log10ws	-9.49		Crippen Method
logp	8.092		Crippen Method
mcvol	368.390	ml/mol	McGowan Method
pc	814.00	kPa	Joback Method
rinpol	2667.00		NIST Webbook
rinpol	2667.00		NIST Webbook
tb	939.67	K	Joback Method
tc	1154.65	K	Joback Method
tf	551.75	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1237.57	J/mol×K	939.67	Joback Method
cpg	1253.73	J/mol×K	975.50	Joback Method
cpg	1268.69	J/mol×K	1011.33	Joback Method
cpg	1282.59	J/mol×K	1047.16	Joback Method
cpg	1295.52	J/mol×K	1082.99	Joback Method
cpg	1307.61	J/mol×K	1118.82	Joback Method
cpg	1318.97	J/mol×K	1154.65	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=U356596&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