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

Inchi: InChI=1S/C27H36F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-38-22(36)20-15-14-16-21(18
InchiKey: FSPYCSSXUSHJPF-UHFFFAOYSA-N
Formula: C27H36F8O4
SMILES: CCCCCCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1
Mol. weight [g/mol]: 576.56

Physical Properties

Property code	Value	Unit	Source
gf	-1741.00	kJ/mol	Joback Method
hf	-2465.56	kJ/mol	Joback Method
hfus	63.79	kJ/mol	Joback Method
hvap	86.13	kJ/mol	Joback Method
log10ws	-10.33		Crippen Method
logp	8.872		Crippen Method
mcvol	396.570	ml/mol	McGowan Method
pc	731.65	kPa	Joback Method
rinpol	2857.00		NIST Webbook
tb	985.43	K	Joback Method
tc	1219.21	K	Joback Method
tf	574.29	K	Joback Method
vc	1.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1360.52	J/mol×K	985.43	Joback Method
cpg	1378.11	J/mol×K	1024.39	Joback Method
cpg	1394.36	J/mol×K	1063.36	Joback Method
cpg	1409.44	J/mol×K	1102.32	Joback Method
cpg	1423.50	J/mol×K	1141.29	Joback Method
cpg	1436.70	J/mol×K	1180.25	Joback Method
cpg	1449.21	J/mol×K	1219.21	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=U356598&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

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