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

Inchi: InChI=1S/C23H28F8O4/c1-2-3-4-5-6-7-8-9-13-34-18(32)16-11-10-12-17(14-16)19(33)35
InchiKey: ZKFCNWDBRPHZIO-UHFFFAOYSA-N
Formula: C23H28F8O4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)c1
Mol. weight [g/mol]: 520.45

Physical Properties

Property code	Value	Unit	Source
gf	-1774.68	kJ/mol	Joback Method
hf	-2383.00	kJ/mol	Joback Method
hfus	53.43	kJ/mol	Joback Method
hvap	77.23	kJ/mol	Joback Method
log10ws	-8.65		Crippen Method
logp	7.312		Crippen Method
mcvol	340.210	ml/mol	McGowan Method
pc	911.08	kPa	Joback Method
rinpol	2476.00		NIST Webbook
tb	893.91	K	Joback Method
tc	1094.78	K	Joback Method
tf	529.21	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1116.93	J/mol×K	893.91	Joback Method
cpg	1131.94	J/mol×K	927.39	Joback Method
cpg	1145.87	J/mol×K	960.87	Joback Method
cpg	1158.81	J/mol×K	994.34	Joback Method
cpg	1170.84	J/mol×K	1027.82	Joback Method
cpg	1182.07	J/mol×K	1061.30	Joback Method
cpg	1192.57	J/mol×K	1094.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356594&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