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

Inchi: InChI=1S/C29H40F8O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-40-24(38)22-17-16-18

InchiKey: SPCKDHHGZIWXHA-UHFFFAOYSA-N

Formula: C29H40F8O4

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

Mol. weight [g/mol]: 604.61

Physical Properties

Property code	Value	Unit	Source
gf	-1724.16	kJ/mol	Joback Method
hf	-2506.84	kJ/mol	Joback Method
hfus	68.97	kJ/mol	Joback Method
hvap	90.59	kJ/mol	Joback Method
log10ws	-11.17		Crippen Method
logp	9.652		Crippen Method
mcvol	424.750	ml/mol	McGowan Method
pc	661.19	kPa	Joback Method
rinpol	3062.00		NIST Webbook
tb	1031.19	K	Joback Method
tc	1289.26	K	Joback Method
tf	596.83	K	Joback Method
vc	1.704	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1485.54	J/mol×K	1031.19	Joback Method
cpg	1504.90	J/mol×K	1074.20	Joback Method
cpg	1522.76	J/mol×K	1117.21	Joback Method
cpg	1539.35	J/mol×K	1160.23	Joback Method
cpg	1554.90	J/mol×K	1203.24	Joback Method
cpg	1569.61	J/mol×K	1246.25	Joback Method
cpg	1583.72	J/mol×K	1289.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356600&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

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