Phthalic acid, pentadecyl pentafluorophenyl ester

Inchi: InChI=1S/C29H35F5O4/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-19-37-28(35)20-17-14-15-18

InchiKey: SVRJQQDXCMLKHX-UHFFFAOYSA-N

Formula: C29H35F5O4

SMILES: CCCCCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 542.58

Physical Properties

Property code	Value	Unit	Source
gf	-1081.55	kJ/mol	Joback Method
hf	-1707.80	kJ/mol	Joback Method
hfus	77.59	kJ/mol	Joback Method
hvap	102.90	kJ/mol	Joback Method
log10ws	-11.32		Crippen Method
logp	8.849		Crippen Method
mcvol	395.680	ml/mol	McGowan Method
pc	787.71	kPa	Joback Method
rinpol	3151.00		NIST Webbook
rinpol	3151.00		NIST Webbook
tb	1095.09	K	Joback Method
tc	1360.30	K	Joback Method
tf	691.82	K	Joback Method
vc	1.581	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1348.25	J/mol×K	1095.09	Joback Method
cpg	1362.10	J/mol×K	1139.29	Joback Method
cpg	1373.70	J/mol×K	1183.49	Joback Method
cpg	1383.14	J/mol×K	1227.70	Joback Method
cpg	1390.49	J/mol×K	1271.90	Joback Method
cpg	1395.81	J/mol×K	1316.10	Joback Method
cpg	1399.17	J/mol×K	1360.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356364&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