Phthalic acid, dodecyl pentafluorophenyl ester

Inchi: InChI=1S/C26H29F5O4/c1-2-3-4-5-6-7-8-9-10-13-16-34-25(32)17-14-11-12-15-18(17)26
InchiKey: ZRFGANAQUQVLKJ-UHFFFAOYSA-N
Formula: C26H29F5O4
SMILES: CCCCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 500.50

Physical Properties

Property code	Value	Unit	Source
gf	-1106.81	kJ/mol	Joback Method
hf	-1645.88	kJ/mol	Joback Method
hfus	69.82	kJ/mol	Joback Method
hvap	96.22	kJ/mol	Joback Method
log10ws	-10.06		Crippen Method
logp	7.679		Crippen Method
mcvol	353.410	ml/mol	McGowan Method
pc	932.35	kPa	Joback Method
rinpol	2830.00		NIST Webbook
rinpol	2830.00		NIST Webbook
tb	1026.45	K	Joback Method
tc	1260.80	K	Joback Method
tf	658.01	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1165.69	J/mol×K	1026.45	Joback Method
cpg	1178.86	J/mol×K	1065.51	Joback Method
cpg	1190.34	J/mol×K	1104.57	Joback Method
cpg	1200.18	J/mol×K	1143.63	Joback Method
cpg	1208.39	J/mol×K	1182.69	Joback Method
cpg	1215.02	J/mol×K	1221.75	Joback Method
cpg	1220.11	J/mol×K	1260.80	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=U356357&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