Phthalic acid, decyl pentafluorophenyl ester

Inchi: InChI=1S/C24H25F5O4/c1-2-3-4-5-6-7-8-11-14-32-23(30)15-12-9-10-13-16(15)24(31)33
InchiKey: JNDYMHBDCQHBOU-UHFFFAOYSA-N
Formula: C24H25F5O4
SMILES: CCCCCCCCCCOC(=O)c1ccccc1C(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 472.44

Physical Properties

Property code	Value	Unit	Source
gf	-1123.65	kJ/mol	Joback Method
hf	-1604.60	kJ/mol	Joback Method
hfus	64.64	kJ/mol	Joback Method
hvap	91.77	kJ/mol	Joback Method
log10ws	-9.23		Crippen Method
logp	6.899		Crippen Method
mcvol	325.230	ml/mol	McGowan Method
pc	1052.09	kPa	Joback Method
rinpol	2644.00		NIST Webbook
rinpol	2644.00		NIST Webbook
tb	980.69	K	Joback Method
tc	1200.93	K	Joback Method
tf	635.47	K	Joback Method
vc	1.302	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1045.74	J/mol×K	980.69	Joback Method
cpg	1058.46	J/mol×K	1017.40	Joback Method
cpg	1069.74	J/mol×K	1054.10	Joback Method
cpg	1079.62	J/mol×K	1090.81	Joback Method
cpg	1088.11	J/mol×K	1127.52	Joback Method
cpg	1095.23	J/mol×K	1164.22	Joback Method
cpg	1101.02	J/mol×K	1200.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U356305&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