Isophthalic acid, decyl pentafluorobenzyl ester

Inchi: InChI=1S/C25H27F5O4/c1-2-3-4-5-6-7-8-9-13-33-24(31)16-11-10-12-17(14-16)25(32)34
InchiKey: ALSZQMIIKHLDFY-UHFFFAOYSA-N
Formula: C25H27F5O4
SMILES: CCCCCCCCCCOC(=O)c1cccc(C(=O)OCc2c(F)c(F)c(F)c(F)c2F)c1
Mol. weight [g/mol]: 486.47

Physical Properties

Property code	Value	Unit	Source
gf	-1115.23	kJ/mol	Joback Method
hf	-1625.24	kJ/mol	Joback Method
hfus	67.23	kJ/mol	Joback Method
hvap	93.99	kJ/mol	Joback Method
log10ws	-9.49		Crippen Method
logp	7.037		Crippen Method
mcvol	339.320	ml/mol	McGowan Method
pc	989.51	kPa	Joback Method
rinpol	3004.00		NIST Webbook
rinpol	3004.00		NIST Webbook
tb	1003.57	K	Joback Method
tc	1230.28	K	Joback Method
tf	646.74	K	Joback Method
vc	1.357	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1105.50	J/mol×K	1003.57	Joback Method
cpg	1118.45	J/mol×K	1041.36	Joback Method
cpg	1129.85	J/mol×K	1079.14	Joback Method
cpg	1139.72	J/mol×K	1116.93	Joback Method
cpg	1148.09	J/mol×K	1154.71	Joback Method
cpg	1155.01	J/mol×K	1192.50	Joback Method
cpg	1160.48	J/mol×K	1230.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344509&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