Isophthalic acid, hexyl pentafluorobenzyl ester

Inchi: InChI=1S/C21H19F5O4/c1-2-3-4-5-9-29-20(27)12-7-6-8-13(10-12)21(28)30-11-14-15(22
InchiKey: RYYOCMFHWXMQSQ-UHFFFAOYSA-N
Formula: C21H19F5O4
SMILES: CCCCCCOC(=O)c1cccc(C(=O)OCc2c(F)c(F)c(F)c(F)c2F)c1
Mol. weight [g/mol]: 430.37

Physical Properties

Property code	Value	Unit	Source
gf	-1148.91	kJ/mol	Joback Method
hf	-1542.68	kJ/mol	Joback Method
hfus	56.87	kJ/mol	Joback Method
hvap	85.09	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	5.476		Crippen Method
mcvol	282.960	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook
tb	912.05	K	Joback Method
tc	1119.10	K	Joback Method
tf	601.66	K	Joback Method
vc	1.133	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.49	J/mol×K	912.05	Joback Method
cpg	881.51	J/mol×K	946.56	Joback Method
cpg	892.37	J/mol×K	981.07	Joback Method
cpg	902.08	J/mol×K	1015.58	Joback Method
cpg	910.65	J/mol×K	1050.09	Joback Method
cpg	918.10	J/mol×K	1084.59	Joback Method
cpg	924.42	J/mol×K	1119.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U344505&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