Isophthalic acid, octyl pentafluorobenzyl ester

Inchi: InChI=1S/C23H23F5O4/c1-2-3-4-5-6-7-11-31-22(29)14-9-8-10-15(12-14)23(30)32-13-16
InchiKey: NXAMEOXJDGBYJQ-UHFFFAOYSA-N
Formula: C23H23F5O4
SMILES: CCCCCCCCOC(=O)c1cccc(C(=O)OCc2c(F)c(F)c(F)c(F)c2F)c1
Mol. weight [g/mol]: 458.42

Physical Properties

Property code	Value	Unit	Source
gf	-1132.07	kJ/mol	Joback Method
hf	-1583.96	kJ/mol	Joback Method
hfus	62.05	kJ/mol	Joback Method
hvap	89.54	kJ/mol	Joback Method
log10ws	-8.65		Crippen Method
logp	6.256		Crippen Method
mcvol	311.140	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2790.00		NIST Webbook
rinpol	2790.00		NIST Webbook
tb	957.81	K	Joback Method
tc	1172.66	K	Joback Method
tf	624.20	K	Joback Method
vc	1.246	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.44	J/mol×K	957.81	Joback Method
cpg	998.93	J/mol×K	993.62	Joback Method
cpg	1010.09	J/mol×K	1029.43	Joback Method
cpg	1019.94	J/mol×K	1065.24	Joback Method
cpg	1028.50	J/mol×K	1101.05	Joback Method
cpg	1035.78	J/mol×K	1136.85	Joback Method
cpg	1041.81	J/mol×K	1172.66	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=U344507&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