1-Butoxypropan-2-yl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C14H15F5O3/c1-3-4-5-21-6-7(2)22-14(20)8-9(15)11(17)13(19)12(18)10(8)16/h

InchiKey: HIPHBAOSIJPGCZ-UHFFFAOYSA-N

Formula: C14H15F5O3

SMILES: CCCCOCC(C)OC(=O)c1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 326.26

Physical Properties

Property code	Value	Unit	Source
gf	-1184.15	kJ/mol	Joback Method
hf	-1515.96	kJ/mol	Joback Method
hfus	39.96	kJ/mol	Joback Method
hvap	59.44	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	3.744		Crippen Method
mcvol	206.520	ml/mol	McGowan Method
pc	1607.71	kPa	Joback Method
rinpol	1521.00		NIST Webbook
rinpol	1521.00		NIST Webbook
tb	665.92	K	Joback Method
tc	838.18	K	Joback Method
tf	418.90	K	Joback Method
vc	0.838	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.19	J/mol×K	665.92	Joback Method
cpg	571.85	J/mol×K	694.63	Joback Method
cpg	583.94	J/mol×K	723.34	Joback Method
cpg	595.44	J/mol×K	752.05	Joback Method
cpg	606.35	J/mol×K	780.76	Joback Method
cpg	616.67	J/mol×K	809.47	Joback Method
cpg	626.40	J/mol×K	838.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378289&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