1-((1-Methoxypropan-2-yl)oxy)propan-2-yl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C14H15F5O4/c1-6(4-21-3)22-5-7(2)23-14(20)8-9(15)11(17)13(19)12(18)10(8)1

InchiKey: QDDPHVROTSKGNV-UHFFFAOYSA-N

Formula: C14H15F5O4

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

Mol. weight [g/mol]: 342.26

Physical Properties

Property code	Value	Unit	Source
gf	-1291.59	kJ/mol	Joback Method
hf	-1653.46	kJ/mol	Joback Method
hfus	37.63	kJ/mol	Joback Method
hvap	61.46	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	2.979		Crippen Method
mcvol	212.390	ml/mol	McGowan Method
pc	1596.17	kPa	Joback Method
rinpol	1566.00		NIST Webbook
tb	687.90	K	Joback Method
tc	862.86	K	Joback Method
tf	426.13	K	Joback Method
vc	0.850	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.36	J/mol×K	687.90	Joback Method
cpg	599.13	J/mol×K	717.06	Joback Method
cpg	611.28	J/mol×K	746.22	Joback Method
cpg	622.79	J/mol×K	775.38	Joback Method
cpg	633.66	J/mol×K	804.54	Joback Method
cpg	643.87	J/mol×K	833.70	Joback Method
cpg	653.40	J/mol×K	862.86	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378290&Units=SI

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

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