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

Inchi: InChI=1S/C17H21F5O4/c1-4-5-6-24-7-9(2)25-8-10(3)26-17(23)11-12(18)14(20)16(22)15

InchiKey: SJACYCMZHNAINQ-UHFFFAOYSA-N

Formula: C17H21F5O4

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

Mol. weight [g/mol]: 384.34

Physical Properties

Property code	Value	Unit	Source
gf	-1266.33	kJ/mol	Joback Method
hf	-1715.38	kJ/mol	Joback Method
hfus	45.40	kJ/mol	Joback Method
hvap	68.14	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.149		Crippen Method
mcvol	254.660	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	1789.00		NIST Webbook
rinpol	1789.00		NIST Webbook
tb	756.54	K	Joback Method
tc	934.13	K	Joback Method
tf	459.94	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.36	J/mol×K	756.54	Joback Method
cpg	764.68	J/mol×K	786.14	Joback Method
cpg	778.20	J/mol×K	815.74	Joback Method
cpg	790.89	J/mol×K	845.34	Joback Method
cpg	802.76	J/mol×K	874.94	Joback Method
cpg	813.79	J/mol×K	904.53	Joback Method
cpg	823.99	J/mol×K	934.13	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=U378291&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