1-(2,2-Dimethyl-1,3-dioxolan-4-yl)-2-methoxy-2-ox
2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C15H13F5O6/c1-15(2)24-4-5(26-15)12(14(22)23-3)25-13(21)6-7(16)9(18)11(2

InchiKey: SRUJXXWXUCZDTP-UHFFFAOYSA-N

Formula: C15H13F5O6

SMILES: COC(=O)C(OC(=O)c1c(F)c(F)c(F)c(F)c1F)C1COC(C)(C)O1

Mol. weight [g/mol]: 384.25

Physical Properties

Property code	Value	Unit	Source
gf	-1453.54	kJ/mol	Joback Method
hf	-1857.80	kJ/mol	Joback Method
hfus	48.82	kJ/mol	Joback Method
hvap	76.23	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	2.232		Crippen Method
mcvol	223.060	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	1759.00		NIST Webbook
rinpol	1759.00		NIST Webbook
tb	807.42	K	Joback Method
tc	1008.39	K	Joback Method
tf	563.80	K	Joback Method
vc	0.879	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.26	J/mol×K	807.42	Joback Method
cpg	691.24	J/mol×K	840.91	Joback Method
cpg	703.70	J/mol×K	874.41	Joback Method
cpg	715.69	J/mol×K	907.90	Joback Method
cpg	727.27	J/mol×K	941.40	Joback Method
cpg	738.50	J/mol×K	974.89	Joback Method
cpg	749.43	J/mol×K	1008.39	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=U373608&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