2,4-Dimethylpentan-3-yl 2,3,4,5,6-pentafluorobenzoate

Inchi: InChI=1S/C14H15F5O2/c1-5(2)13(6(3)4)21-14(20)7-8(15)10(17)12(19)11(18)9(7)16/h5-6

InchiKey: PDADNVLCYCMZTB-UHFFFAOYSA-N

Formula: C14H15F5O2

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

Mol. weight [g/mol]: 310.26

Physical Properties

Property code	Value	Unit	Source
gf	-1084.03	kJ/mol	Joback Method
hf	-1394.30	kJ/mol	Joback Method
hfus	31.73	kJ/mol	Joback Method
hvap	56.25	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.220		Crippen Method
mcvol	200.650	ml/mol	McGowan Method
pc	1651.11	kPa	Joback Method
rinpol	1406.00		NIST Webbook
rinpol	1406.00		NIST Webbook
tb	642.62	K	Joback Method
tc	819.55	K	Joback Method
tf	366.67	K	Joback Method
vc	0.807	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	533.65	J/mol×K	642.62	Joback Method
cpg	546.84	J/mol×K	672.11	Joback Method
cpg	559.41	J/mol×K	701.60	Joback Method
cpg	571.37	J/mol×K	731.08	Joback Method
cpg	582.71	J/mol×K	760.57	Joback Method
cpg	593.44	J/mol×K	790.06	Joback Method
cpg	603.55	J/mol×K	819.55	Joback Method

Sources

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=U373689&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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