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

Inchi: InChI=1S/C13H13F5O2/c1-5(2)4-6(3)20-13(19)7-8(14)10(16)12(18)11(17)9(7)15/h5-6H,4

InchiKey: LSAKNAZPUHYCEQ-UHFFFAOYSA-N

Formula: C13H13F5O2

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

Mol. weight [g/mol]: 296.23

Physical Properties

Property code	Value	Unit	Source
gf	-1090.01	kJ/mol	Joback Method
hf	-1368.38	kJ/mol	Joback Method
hfus	32.66	kJ/mol	Joback Method
hvap	54.41	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	3.974		Crippen Method
mcvol	186.560	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	1318.00		NIST Webbook
tb	620.18	K	Joback Method
tc	795.32	K	Joback Method
tf	370.40	K	Joback Method
vc	0.757	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.63	J/mol×K	620.18	Joback Method
cpg	494.95	J/mol×K	649.37	Joback Method
cpg	506.72	J/mol×K	678.56	Joback Method
cpg	517.94	J/mol×K	707.75	Joback Method
cpg	528.61	J/mol×K	736.94	Joback Method
cpg	538.73	J/mol×K	766.13	Joback Method
cpg	548.31	J/mol×K	795.32	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=U373690&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