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

Inchi: InChI=1S/C13H13F5O2/c1-4-13(3,5-2)20-12(19)6-7(14)9(16)11(18)10(17)8(6)15/h4-5H2

InchiKey: AVHDRMHRBXEPHW-UHFFFAOYSA-N

Formula: C13H13F5O2

SMILES: CCC(C)(CC)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	-1082.29	kJ/mol	Joback Method
hf	-1366.57	kJ/mol	Joback Method
hfus	32.29	kJ/mol	Joback Method
hvap	53.89	kJ/mol	Joback Method
log10ws	-5.58		Crippen Method
logp	4.118		Crippen Method
mcvol	186.560	ml/mol	McGowan Method
pc	1780.34	kPa	Joback Method
rinpol	1350.00		NIST Webbook
tb	617.83	K	Joback Method
tc	795.18	K	Joback Method
tf	402.82	K	Joback Method
vc	0.758	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	484.99	J/mol×K	617.83	Joback Method
cpg	497.28	J/mol×K	647.39	Joback Method
cpg	508.96	J/mol×K	676.95	Joback Method
cpg	520.05	J/mol×K	706.51	Joback Method
cpg	530.56	J/mol×K	736.07	Joback Method
cpg	540.50	J/mol×K	765.62	Joback Method
cpg	549.88	J/mol×K	795.18	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=U373688&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