Pentafluorobenzoic acid, but-3-yn-2-yl ester

Inchi: InChI=1S/C11H5F5O2/c1-3-4(2)18-11(17)5-6(12)8(14)10(16)9(15)7(5)13/h1,4H,2H3
InchiKey: KWGBKJUEKIANIM-UHFFFAOYSA-N
Formula: C11H5F5O2
SMILES: C#CC(C)OC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 264.15

Physical Properties

Property code	Value	Unit	Source
gf	-881.34	kJ/mol	Joback Method
hf	-1029.92	kJ/mol	Joback Method
hfus	33.98	kJ/mol	Joback Method
hvap	50.21	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	2.561		Crippen Method
mcvol	149.780	ml/mol	McGowan Method
pc	2400.57	kPa	Joback Method
rinpol	1020.00		NIST Webbook
tb	564.98	K	Joback Method
tc	749.60	K	Joback Method
tf	409.83	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.51	J/mol×K	564.98	Joback Method
cpg	356.65	J/mol×K	595.75	Joback Method
cpg	365.39	J/mol×K	626.52	Joback Method
cpg	373.72	J/mol×K	657.29	Joback Method
cpg	381.63	J/mol×K	688.06	Joback Method
cpg	389.14	J/mol×K	718.83	Joback Method
cpg	396.23	J/mol×K	749.60	Joback Method

Sources

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=U299181&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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