Pentafluorobenzoic acid, hex-4-yn-3-yl ester

Inchi: InChI=1S/C13H9F5O2/c1-3-5-6(4-2)20-13(19)7-8(14)10(16)12(18)11(17)9(7)15/h6H,4H2
InchiKey: ZBEFRKYTRGWTFP-UHFFFAOYSA-N
Formula: C13H9F5O2
SMILES: CC#CC(CC)OC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 292.20

Physical Properties

Property code	Value	Unit	Source
gf	-884.77	kJ/mol	Joback Method
hf	-1090.80	kJ/mol	Joback Method
hfus	39.31	kJ/mol	Joback Method
hvap	56.95	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	3.341		Crippen Method
mcvol	177.960	ml/mol	McGowan Method
pc	2027.23	kPa	Joback Method
rinpol	1388.00		NIST Webbook
tb	629.62	K	Joback Method
tc	818.87	K	Joback Method
tf	491.50	K	Joback Method
vc	0.726	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	440.54	J/mol×K	629.62	Joback Method
cpg	451.80	J/mol×K	661.16	Joback Method
cpg	462.52	J/mol×K	692.70	Joback Method
cpg	472.71	J/mol×K	724.24	Joback Method
cpg	482.36	J/mol×K	755.79	Joback Method
cpg	491.47	J/mol×K	787.33	Joback Method
cpg	500.03	J/mol×K	818.87	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=U299184&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