Pentafluorobenzoic acid, pent-2-en-4-ynyl ester

Inchi: InChI=1S/C12H5F5O2/c1-2-3-4-5-19-12(18)6-7(13)9(15)11(17)10(16)8(6)14/h1,3-4H,5H

InchiKey: YDOVTBUPHCWONQ-UHFFFAOYSA-N

Formula: C12H5F5O2

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

Mol. weight [g/mol]: 276.16

Physical Properties

Property code	Value	Unit	Source
gf	-790.26	kJ/mol	Joback Method
hf	-928.06	kJ/mol	Joback Method
hfus	40.30	kJ/mol	Joback Method
hvap	52.78	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	2.728		Crippen Method
mcvol	159.570	ml/mol	McGowan Method
pc	2282.77	kPa	Joback Method
rinpol	1360.00		NIST Webbook
rinpol	1360.00		NIST Webbook
tb	592.46	K	Joback Method
tc	778.90	K	Joback Method
tf	431.02	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	371.96	J/mol×K	592.46	Joback Method
cpg	381.18	J/mol×K	623.53	Joback Method
cpg	389.93	J/mol×K	654.61	Joback Method
cpg	398.23	J/mol×K	685.68	Joback Method
cpg	406.08	J/mol×K	716.75	Joback Method
cpg	413.51	J/mol×K	747.83	Joback Method
cpg	420.52	J/mol×K	778.90	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=U299183&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