Prop-2-ynyl 2,3,4,5,6-pentafluorobenzoate

Other names: 2-propynyl pentaflurobenzoate
Inchi: InChI=1S/C10H3F5O2/c1-2-3-17-10(16)4-5(11)7(13)9(15)8(14)6(4)12/h1H,3H2
InchiKey: CHIDSPLDGZHPMC-UHFFFAOYSA-N
Formula: C10H3F5O2
SMILES: C#CCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 250.12

Physical Properties

Property code	Value	Unit	Source
gf	-887.32	kJ/mol	Joback Method
hf	-1004.00	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	48.37	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	2.172		Crippen Method
mcvol	135.690	ml/mol	McGowan Method
pc	2621.78	kPa	Joback Method
rinpol	1122.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1107.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1123.00		NIST Webbook
ripol	1664.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1676.00		NIST Webbook
ripol	1682.00		NIST Webbook
ripol	1688.00		NIST Webbook
tb	542.54	K	Joback Method
tc	725.57	K	Joback Method
tf	413.56	K	Joback Method
vc	0.564	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.55	J/mol×K	542.54	Joback Method
cpg	311.47	J/mol×K	573.05	Joback Method
cpg	319.06	J/mol×K	603.55	Joback Method
cpg	326.32	J/mol×K	634.06	Joback Method
cpg	333.24	J/mol×K	664.56	Joback Method
cpg	339.82	J/mol×K	695.07	Joback Method
cpg	346.06	J/mol×K	725.57	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=U373686&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume