Carbonic acid, allyl pentafluorobenzyl ester

Inchi: InChI=1S/C11H7F5O3/c1-2-3-18-11(17)19-4-5-6(12)8(14)10(16)9(15)7(5)13/h2H,1,3-4H
InchiKey: PIIYRRIKWCTTOL-UHFFFAOYSA-N
Formula: C11H7F5O3
SMILES: C=CCOC(=O)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 282.16

Physical Properties

Property code	Value	Unit	Source
gf	-1119.13	kJ/mol	Joback Method
hf	-1323.33	kJ/mol	Joback Method
hfus	34.44	kJ/mol	Joback Method
hvap	52.48	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.221		Crippen Method
mcvol	159.950	ml/mol	McGowan Method
pc	2119.73	kPa	Joback Method
rinpol	1325.00		NIST Webbook
rinpol	1325.00		NIST Webbook
tb	594.40	K	Joback Method
tc	768.25	K	Joback Method
tf	398.33	K	Joback Method
vc	0.656	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	388.72	J/mol×K	594.40	Joback Method
cpg	398.41	J/mol×K	623.37	Joback Method
cpg	407.71	J/mol×K	652.35	Joback Method
cpg	416.61	J/mol×K	681.32	Joback Method
cpg	425.10	J/mol×K	710.30	Joback Method
cpg	433.18	J/mol×K	739.27	Joback Method
cpg	440.83	J/mol×K	768.25	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=U357379&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume