Carbonic acid, propargyl 3,5-difluophenyl ester

Inchi: InChI=1S/C10H6F2O3/c1-2-3-14-10(13)15-9-5-7(11)4-8(12)6-9/h1,4-6H,3H2
InchiKey: DFPDNMFLPHKJON-UHFFFAOYSA-N
Formula: C10H6F2O3
SMILES: C#CCOC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 212.15

Physical Properties

Property code	Value	Unit	Source
gf	-379.00	kJ/mol	Joback Method
hf	-513.48	kJ/mol	Joback Method
hfus	28.03	kJ/mol	Joback Method
hvap	51.24	kJ/mol	Joback Method
log10ws	-3.15		Crippen Method
logp	2.113		Crippen Method
mcvol	136.250	ml/mol	McGowan Method
pc	3121.00	kPa	Joback Method
rinpol	1249.00		NIST Webbook
rinpol	1249.00		NIST Webbook
tb	552.21	K	Joback Method
tc	758.28	K	Joback Method
tf	396.46	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.59	J/mol×K	552.21	Joback Method
cpg	312.62	J/mol×K	586.55	Joback Method
cpg	322.14	J/mol×K	620.90	Joback Method
cpg	331.15	J/mol×K	655.24	Joback Method
cpg	339.65	J/mol×K	689.59	Joback Method
cpg	347.64	J/mol×K	723.93	Joback Method
cpg	355.12	J/mol×K	758.28	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=U357907&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