Carbonic acid, allyl 3-fluorophenyl ester

Inchi: InChI=1S/C10H9FO3/c1-2-6-13-10(12)14-9-5-3-4-8(11)7-9/h2-5,7H,1,6H2
InchiKey: KCEGDOSJRRNENM-UHFFFAOYSA-N
Formula: C10H9FO3
SMILES: C=CCOC(=O)Oc1cccc(F)c1
Mol. weight [g/mol]: 196.18

Physical Properties

Property code	Value	Unit	Source
gf	-309.79	kJ/mol	Joback Method
hf	-472.37	kJ/mol	Joback Method
hfus	21.08	kJ/mol	Joback Method
hvap	50.87	kJ/mol	Joback Method
log10ws	-2.87		Crippen Method
logp	2.527		Crippen Method
mcvol	138.780	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
rinpol	1277.00		NIST Webbook
tb	554.52	K	Joback Method
tc	760.03	K	Joback Method
tf	334.62	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.81	J/mol×K	554.52	Joback Method
cpg	324.52	J/mol×K	588.77	Joback Method
cpg	335.61	J/mol×K	623.02	Joback Method
cpg	346.10	J/mol×K	657.27	Joback Method
cpg	355.98	J/mol×K	691.53	Joback Method
cpg	365.27	J/mol×K	725.78	Joback Method
cpg	373.95	J/mol×K	760.03	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=U357378&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