Carbonic acid, ethyl 3,5-difluophenyl ester

Inchi: InChI=1S/C9H8F2O3/c1-2-13-9(12)14-8-4-6(10)3-7(11)5-8/h3-5H,2H2,1H3
InchiKey: JNQNBNWVOCKDKL-UHFFFAOYSA-N
Formula: C9H8F2O3
SMILES: CCOC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 202.15

Physical Properties

Property code	Value	Unit	Source
gf	-610.49	kJ/mol	Joback Method
hf	-784.74	kJ/mol	Joback Method
hfus	22.46	kJ/mol	Joback Method
hvap	49.16	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.500		Crippen Method
mcvol	130.760	ml/mol	McGowan Method
pc	2947.28	kPa	Joback Method
rinpol	1169.00		NIST Webbook
rinpol	1169.00		NIST Webbook
tb	539.21	K	Joback Method
tc	734.87	K	Joback Method
tf	338.22	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	295.10	J/mol×K	539.21	Joback Method
cpg	305.69	J/mol×K	571.82	Joback Method
cpg	315.81	J/mol×K	604.43	Joback Method
cpg	325.47	J/mol×K	637.04	Joback Method
cpg	334.66	J/mol×K	669.65	Joback Method
cpg	343.36	J/mol×K	702.26	Joback Method
cpg	351.57	J/mol×K	734.87	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=U357912&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