Carbonic acid, isobutyl 3,5-difluophenyl ester

Inchi: InChI=1S/C11H12F2O3/c1-7(2)6-15-11(14)16-10-4-8(12)3-9(13)5-10/h3-5,7H,6H2,1-2H3
InchiKey: ZMJNKEALKFWQLQ-UHFFFAOYSA-N
Formula: C11H12F2O3
SMILES: CC(C)COC(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 230.21

Physical Properties

Property code	Value	Unit	Source
gf	-596.09	kJ/mol	Joback Method
hf	-831.30	kJ/mol	Joback Method
hfus	24.12	kJ/mol	Joback Method
hvap	53.22	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.136		Crippen Method
mcvol	158.940	ml/mol	McGowan Method
pc	2436.25	kPa	Joback Method
rinpol	1284.00		NIST Webbook
tb	584.53	K	Joback Method
tc	778.96	K	Joback Method
tf	345.76	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	387.09	J/mol×K	584.53	Joback Method
cpg	399.79	J/mol×K	616.94	Joback Method
cpg	411.87	J/mol×K	649.34	Joback Method
cpg	423.34	J/mol×K	681.75	Joback Method
cpg	434.19	J/mol×K	714.15	Joback Method
cpg	444.43	J/mol×K	746.56	Joback Method
cpg	454.05	J/mol×K	778.96	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=U357826&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