Carbonic acid, 2-chloroethyl 3,5-difluophenyl ester

Inchi: InChI=1S/C9H7ClF2O3/c10-1-2-14-9(13)15-8-4-6(11)3-7(12)5-8/h3-5H,1-2H2

InchiKey: CNBVZHSPHGTRFU-UHFFFAOYSA-N

Formula: C9H7ClF2O3

SMILES: O=C(OCCCl)Oc1cc(F)cc(F)c1

Mol. weight [g/mol]: 236.60

Physical Properties

Property code	Value	Unit	Source
gf	-622.42	kJ/mol	Joback Method
hf	-800.48	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	53.55	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.719		Crippen Method
mcvol	143.000	ml/mol	McGowan Method
pc	2832.35	kPa	Joback Method
rinpol	1411.00		NIST Webbook
rinpol	1411.00		NIST Webbook
tb	576.64	K	Joback Method
tc	776.80	K	Joback Method
tf	368.14	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.95	J/mol×K	576.64	Joback Method
cpg	328.97	J/mol×K	610.00	Joback Method
cpg	338.50	J/mol×K	643.36	Joback Method
cpg	347.51	J/mol×K	676.72	Joback Method
cpg	356.01	J/mol×K	710.08	Joback Method
cpg	364.00	J/mol×K	743.44	Joback Method
cpg	371.46	J/mol×K	776.80	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=U357879&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