2-Chloropropionic acid, 3,5-difluophenyl ester

Inchi: InChI=1S/C9H7ClF2O2/c1-5(10)9(13)14-8-3-6(11)2-7(12)4-8/h2-5H,1H3
InchiKey: IKRUDTQLJRNXAM-UHFFFAOYSA-N
Formula: C9H7ClF2O2
SMILES: CC(Cl)C(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 220.60

Physical Properties

Property code	Value	Unit	Source
gf	-519.86	kJ/mol	Joback Method
hf	-673.54	kJ/mol	Joback Method
hfus	21.95	kJ/mol	Joback Method
hvap	50.75	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.498		Crippen Method
mcvol	137.130	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1234.00		NIST Webbook
tb	553.78	K	Joback Method
tc	760.06	K	Joback Method
tf	330.91	K	Joback Method
vc	0.534	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	297.10	J/mol×K	553.78	Joback Method
cpg	307.49	J/mol×K	588.16	Joback Method
cpg	317.30	J/mol×K	622.54	Joback Method
cpg	326.56	J/mol×K	656.92	Joback Method
cpg	335.26	J/mol×K	691.30	Joback Method
cpg	343.40	J/mol×K	725.68	Joback Method
cpg	351.01	J/mol×K	760.06	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=U357774&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