4-Chlorobutyric acid, 3,5-difluophenyl ester

Inchi: InChI=1S/C10H9ClF2O2/c11-3-1-2-10(14)15-9-5-7(12)4-8(13)6-9/h4-6H,1-3H2
InchiKey: PHNMZHONLSFAFU-UHFFFAOYSA-N
Formula: C10H9ClF2O2
SMILES: O=C(CCCCl)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 234.63

Physical Properties

Property code	Value	Unit	Source
gf	-509.00	kJ/mol	Joback Method
hf	-688.90	kJ/mol	Joback Method
hfus	28.06	kJ/mol	Joback Method
hvap	53.36	kJ/mol	Joback Method
log10ws	-3.44		Crippen Method
logp	2.889		Crippen Method
mcvol	151.220	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1471.00		NIST Webbook
tb	577.10	K	Joback Method
tc	776.22	K	Joback Method
tf	357.18	K	Joback Method
vc	0.597	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	341.72	J/mol×K	577.10	Joback Method
cpg	352.76	J/mol×K	610.29	Joback Method
cpg	363.20	J/mol×K	643.47	Joback Method
cpg	373.07	J/mol×K	676.66	Joback Method
cpg	382.36	J/mol×K	709.85	Joback Method
cpg	391.09	J/mol×K	743.03	Joback Method
cpg	399.27	J/mol×K	776.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357767&Units=SI
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

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