3-Aminobutanoic acid, N-chlorodifluoroacetyl-, ethyl ester

Inchi: InChI=1S/C8H12ClF2NO3/c1-3-15-6(13)4-5(2)12-7(14)8(9,10)11/h5H,3-4H2,1-2H3,(H,12

InchiKey: BNMLRMKMRHPUHB-UHFFFAOYSA-N

Formula: C8H12ClF2NO3

SMILES: CCOC(=O)CC(C)NC(=O)C(F)(F)Cl

Mol. weight [g/mol]: 243.64

Physical Properties

Property code	Value	Unit	Source
gf	-658.12	kJ/mol	Joback Method
hf	-934.35	kJ/mol	Joback Method
hfus	25.38	kJ/mol	Joback Method
hvap	56.81	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.276		Crippen Method
mcvol	158.350	ml/mol	McGowan Method
pc	2592.49	kPa	Joback Method
rinpol	1280.00		NIST Webbook
tb	595.07	K	Joback Method
tc	783.02	K	Joback Method
tf	373.19	K	Joback Method
vc	0.617	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.66	J/mol×K	595.07	Joback Method
cpg	402.64	J/mol×K	626.39	Joback Method
cpg	412.97	J/mol×K	657.72	Joback Method
cpg	422.68	J/mol×K	689.04	Joback Method
cpg	431.79	J/mol×K	720.37	Joback Method
cpg	440.32	J/mol×K	751.69	Joback Method
cpg	448.29	J/mol×K	783.02	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375774&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

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