Benzoic acid, p-(2-chloroacetamido)-, ethyl ester

Inchi: InChI=1S/C11H12ClNO3/c1-2-16-11(15)8-3-5-9(6-4-8)13-10(14)7-12/h3-6H,2,7H2,1H3,(

InchiKey: ZVRJEYAQESBSSH-UHFFFAOYSA-N

Formula: C11H12ClNO3

SMILES: CCOC(=O)c1ccc(NC(=O)CCl)cc1

Mol. weight [g/mol]: 241.67

CAS: 26226-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-140.86	kJ/mol	Joback Method
hf	-364.96	kJ/mol	Joback Method
hfus	31.58	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.041		Crippen Method
mcvol	173.320	ml/mol	McGowan Method
pc	2850.52	kPa	Joback Method
tb	700.50	K	Joback Method
tc	920.59	K	Joback Method
tf	457.34	K	Joback Method
vc	0.657	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.17	J/mol×K	700.50	Joback Method
cpg	446.82	J/mol×K	737.18	Joback Method
cpg	457.63	J/mol×K	773.86	Joback Method
cpg	467.62	J/mol×K	810.55	Joback Method
cpg	476.82	J/mol×K	847.23	Joback Method
cpg	485.23	J/mol×K	883.91	Joback Method
cpg	492.89	J/mol×K	920.59	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26226722&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume