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

Inchi: InChI=1S/C11H12INO3/c1-2-16-11(15)8-3-5-9(6-4-8)13-10(14)7-12/h3-6H,2,7H2,1H3,(H
InchiKey: TZYCRJNOEXMIEG-UHFFFAOYSA-N
Formula: C11H12INO3
SMILES: CCOC(=O)c1ccc(NC(=O)CI)cc1
Mol. weight [g/mol]: 333.12
CAS: 116465-51-1

Physical Properties

Property code	Value	Unit	Source
gf	-70.81	kJ/mol	Joback Method
hf	-272.35	kJ/mol	Joback Method
hfus	31.79	kJ/mol	Joback Method
hvap	74.73	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.237		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	756.21	K	Joback Method
tc	996.12	K	Joback Method
tf	485.48	K	Joback Method
vc	0.697	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.16	J/mol×K	756.21	Joback Method
cpg	465.17	J/mol×K	796.19	Joback Method
cpg	475.27	J/mol×K	836.18	Joback Method
cpg	484.49	J/mol×K	876.16	Joback Method
cpg	492.86	J/mol×K	916.15	Joback Method
cpg	500.44	J/mol×K	956.13	Joback Method
cpg	507.24	J/mol×K	996.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116465511&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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