Carbamic acid, 4-iodophenyl, ethyl ester

Inchi: InChI=1S/C9H10INO2/c1-2-13-9(12)11-8-5-3-7(10)4-6-8/h3-6H,2H2,1H3,(H,11,12)
InchiKey: JUQOQFNQIBKYRA-UHFFFAOYSA-N
Formula: C9H10INO2
SMILES: CCOC(=O)Nc1ccc(I)cc1
Mol. weight [g/mol]: 291.09
CAS: 77774-39-1

Physical Properties

Property code	Value	Unit	Source
gf	41.27	kJ/mol	Joback Method
hf	-118.49	kJ/mol	Joback Method
hfus	25.01	kJ/mol	Joback Method
hvap	63.53	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.860		Crippen Method
mcvol	157.150	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
rinpol	1776.00		NIST Webbook
rinpol	1790.00		NIST Webbook
tb	656.58	K	Joback Method
tc	901.16	K	Joback Method
tf	413.01	K	Joback Method
vc	0.579	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	345.24	J/mol×K	656.58	Joback Method
cpg	356.49	J/mol×K	697.34	Joback Method
cpg	366.90	J/mol×K	738.11	Joback Method
cpg	376.48	J/mol×K	778.87	Joback Method
cpg	385.28	J/mol×K	819.63	Joback Method
cpg	393.33	J/mol×K	860.39	Joback Method
cpg	400.66	J/mol×K	901.16	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C77774391&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