Ethyl 4-iodobenzoate

Other names: p-Iodobenzoic acid ethyl ester
Benzoic acid, 4-iodo-, ethyl ester
Inchi: InChI=1S/C9H9IO2/c1-2-12-9(11)7-3-5-8(10)6-4-7/h3-6H,2H2,1H3
InchiKey: YCBJOQUNPLTBGG-UHFFFAOYSA-N
Formula: C9H9IO2
SMILES: CCOC(=O)c1ccc(I)cc1
Mol. weight [g/mol]: 276.07
CAS: 51934-41-9

Physical Properties

Property code	Value	Unit	Source
gf	-48.12	kJ/mol	Joback Method
hf	-171.96	kJ/mol	Joback Method
hfus	19.91	kJ/mol	Joback Method
hvap	57.09	kJ/mol	Joback Method
log10ws	-3.28		Crippen Method
logp	2.468		Crippen Method
mcvol	147.170	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
tb	606.41	K	Joback Method
tc	853.85	K	Joback Method
tf	360.35	K	Joback Method
vc	0.543	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.70	J/mol×K	606.41	Joback Method
cpg	312.05	J/mol×K	647.65	Joback Method
cpg	322.58	J/mol×K	688.89	Joback Method
cpg	332.32	J/mol×K	730.13	Joback Method
cpg	341.31	J/mol×K	771.37	Joback Method
cpg	349.57	J/mol×K	812.61	Joback Method
cpg	357.13	J/mol×K	853.85	Joback Method

dvisc	0.0018898	Pa×s	360.35	Joback Method
dvisc	0.0011140	Pa×s	401.36	Joback Method
dvisc	0.0007243	Pa×s	442.37	Joback Method
dvisc	0.0005066	Pa×s	483.38	Joback Method
dvisc	0.0003748	Pa×s	524.39	Joback Method
dvisc	0.0002896	Pa×s	565.40	Joback Method
dvisc	0.0002317	Pa×s	606.41	Joback Method

Sources

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=C51934419&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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