

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
mvol	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	m ³ /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	Paxs	360.35	Joback Method
dvisc	0.0011140	Paxs	401.36	Joback Method
dvisc	0.0007243	Paxs	442.37	Joback Method
dvisc	0.0005066	Paxs	483.38	Joback Method
dvisc	0.0003748	Paxs	524.39	Joback Method
dvisc	0.0002896	Paxs	565.40	Joback Method
dvisc	0.0002317	Paxs	606.41	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C51934419&Units=SI

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

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