Ethyl 3-iodobenzoate

Other names: Benzoic acid, 3-iodo-, ethyl ester
Inchi: InChI=1S/C9H9IO2/c1-2-12-9(11)7-4-3-5-8(10)6-7/h3-6H,2H2,1H3
InchiKey: POGCXCWRMMXDAQ-UHFFFAOYSA-N
Formula: C9H9IO2
SMILES: CCOC(=O)c1cccc(I)c1
Mol. weight [g/mol]: 276.07
CAS: 58313-23-8

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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	438.70	K	3.20	NIST Webbook
tbrp	423.20	K	2.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C58313238&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
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
tbrp: Boiling point at reduced pressure

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume