3-Buten-2-one, 4-(2-iodophenyl)-

Other names: o-Iodobenzalacetone
E)-4-(2-Iodophenyl)but-3-en-2-one
4-(2-Iodophenyl)but-3-en-2-one
2-Iodo-benzalacetone
Inchi: InChI=1S/C10H9IO/c1-8(12)6-7-9-4-2-3-5-10(9)11/h2-7H,1H3/b7-6+
InchiKey: VXNAUKLNYVAOKD-VOTSOKGWSA-N
Formula: C10H9IO
SMILES: CC(=O)C=Cc1ccccc1I
Mol. weight [g/mol]: 272.08
CAS: 76293-36-2

Physical Properties

Property code	Value	Unit	Source
gf	145.52	kJ/mol	Joback Method
hf	56.84	kJ/mol	Joback Method
hfus	21.52	kJ/mol	Joback Method
hvap	56.87	kJ/mol	Joback Method
ie	8.30	eV	NIST Webbook
ie	8.60 ± 0.05	eV	NIST Webbook
log10ws	-3.56		Crippen Method
logp	2.893		Crippen Method
mcvol	151.090	ml/mol	McGowan Method
pc	3195.54	kPa	Joback Method
tb	611.03	K	Joback Method
tc	868.38	K	Joback Method
tf	344.31	K	Joback Method
vc	0.561	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	303.29	J/mol×K	611.03	Joback Method
cpg	314.98	J/mol×K	653.92	Joback Method
cpg	325.70	J/mol×K	696.81	Joback Method

cpg	335.53	J/mol×K	739.71	Joback Method
cpg	344.56	J/mol×K	782.60	Joback Method
cpg	352.88	J/mol×K	825.49	Joback Method
cpg	360.58	J/mol×K	868.38	Joback Method
dvisc	0.0022563	Pa×s	344.31	Joback Method
dvisc	0.0012361	Pa×s	388.76	Joback Method
dvisc	0.0007662	Pa×s	433.22	Joback Method
dvisc	0.0005191	Pa×s	477.67	Joback Method
dvisc	0.0003758	Pa×s	522.12	Joback Method
dvisc	0.0002863	Pa×s	566.58	Joback Method
dvisc	0.0002268	Pa×s	611.03	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=C76293362&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
ie: Ionization energy
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