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

Other names: o-Bromobenzalacetone
2-Bromo-benzalacetone
Inchi: InChI=1S/C10H9BrO/c1-8(12)6-7-9-4-2-3-5-10(9)11/h2-7H,1H3/b7-6+
InchiKey: YEXZDFFGPWZWBU-VOTSOKGWSA-N
Formula: C10H9BrO
SMILES: CC(=O)C=Cc1ccccc1Br
Mol. weight [g/mol]: 225.08
CAS: 72454-54-7

Physical Properties

Property code	Value	Unit	Source
gf	101.72	kJ/mol	Joback Method
hf	6.30	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hvap	53.93	kJ/mol	Joback Method
ie	8.70 ± 0.10	eV	NIST Webbook
ie	8.70 ± 0.05	eV	NIST Webbook
ie	8.70 ± 0.05	eV	NIST Webbook
log10ws	-3.58		Crippen Method
logp	3.051		Crippen Method
mcvol	142.770	ml/mol	McGowan Method
pc	3551.53	kPa	Joback Method
tb	584.05	K	Joback Method
tc	824.96	K	Joback Method
tf	346.05	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	293.69	J/mol×K	584.05	Joback Method
cpg	305.48	J/mol×K	624.20	Joback Method
cpg	316.36	J/mol×K	664.35	Joback Method
cpg	326.39	J/mol×K	704.51	Joback Method

cpg	335.66	J/mol×K	744.66	Joback Method
cpg	344.23	J/mol×K	784.81	Joback Method
cpg	352.17	J/mol×K	824.96	Joback Method
dvisc	0.0017851	Pa×s	346.05	Joback Method
dvisc	0.0010639	Pa×s	385.72	Joback Method
dvisc	0.0006984	Pa×s	425.38	Joback Method
dvisc	0.0004925	Pa×s	465.05	Joback Method
dvisc	0.0003670	Pa×s	504.72	Joback Method
dvisc	0.0002854	Pa×s	544.38	Joback Method
dvisc	0.0002297	Pa×s	584.05	Joback Method

Sources

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=C72454547&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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