2-Propen-1-one, 1-(4-bromophenyl)-3-phenyl-

Other names: Chalcone, 4'-bromo-
4'-Bromochalcone
Alpha-benzylidene-p-bromo-acetophenone
1-(4-Bromophenyl)-3-phenyl-2-propen-1-one
Inchi: InChI=1S/C15H11BrO/c16-14-9-7-13(8-10-14)15(17)11-6-12-4-2-1-3-5-12/h1-11H/b11-6
InchiKey: QMHDTKUBDZUMNH-IZZDOVSWSA-N
Formula: C15H11BrO
SMILES: O=C(C=Cc1ccccc1)c1ccc(Br)cc1
Mol. weight [g/mol]: 287.15
CAS: 2403-27-2

Physical Properties

Property code	Value	Unit	Source
gf	256.23	kJ/mol	Joback Method
hf	139.63	kJ/mol	Joback Method
hfus	29.39	kJ/mol	Joback Method
hvap	67.34	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	4.345		Crippen Method
mcvol	189.460	ml/mol	McGowan Method
pc	2995.87	kPa	Joback Method
tb	725.13	K	Joback Method
tc	988.64	K	Joback Method
tf	428.82	K	Joback Method
vc	0.708	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.99	J/mol×K	725.13	Joback Method
cpg	466.44	J/mol×K	769.05	Joback Method
cpg	478.69	J/mol×K	812.97	Joback Method
cpg	489.88	J/mol×K	856.89	Joback Method
cpg	500.14	J/mol×K	900.81	Joback Method

cpg	509.61	J/mol×K	944.73	Joback Method
cpg	518.42	J/mol×K	988.64	Joback Method
dvisc	0.0011601	Pa×s	428.82	Joback Method
dvisc	0.0006755	Pa×s	478.20	Joback Method
dvisc	0.0004353	Pa×s	527.59	Joback Method
dvisc	0.0003024	Pa×s	576.98	Joback Method
dvisc	0.0002225	Pa×s	626.36	Joback Method
dvisc	0.0001712	Pa×s	675.75	Joback Method
dvisc	0.0001365	Pa×s	725.13	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=C2403272&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.