Benzyl 4-bromophenyl ketone

Other names: Benzyl 4-bromophenyl ketone
Ethanone, 1-(4-bromophenyl)-2-phenyl-
Inchi: InChI=1S/C14H11BrO/c15-13-8-6-12(7-9-13)14(16)10-11-4-2-1-3-5-11/h1-9H,10H2
InchiKey: MOSIKPSTRPODHQ-UHFFFAOYSA-N
Formula: C14H11BrO
SMILES: O=C(Cc1ccccc1)c1ccc(Br)cc1
Mol. weight [g/mol]: 275.14

Physical Properties

Property code	Value	Unit	Source
hf	44.30	kJ/mol	Cheméo Relay (1.0)
hfus	26.59	kJ/mol	Joback Method
hvap	89.05	kJ/mol	Cheméo Relay (1.0)
ie	8.66	eV	Cheméo Relay (1.0)
log10ws	-4.65		Cheméo Relay (1.0)
logp	3.874		Crippen Method
mcvol	179.670	ml/mol	McGowan Method
pc	3145.56	kPa	Joback Method
tb	625.90	K	Cheméo Relay (1.0)
tf	362.31	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	426.04	J/mol×K	698.09	Joback Method
cpg	439.70	J/mol×K	741.25	Joback Method
cpg	452.15	J/mol×K	784.41	Joback Method
cpg	463.48	J/mol×K	827.56	Joback Method
cpg	473.80	J/mol×K	870.72	Joback Method
cpg	483.20	J/mol×K	913.88	Joback Method
cpg	491.77	J/mol×K	957.04	Joback Method
dvisc	0.0013511	Pa×s	422.63	Joback Method
dvisc	0.0008160	Pa×s	468.54	Joback Method
dvisc	0.0005392	Pa×s	514.45	Joback Method

dvisc	0.0003813	Pa×s	560.36	Joback Method
dvisc	0.0002842	Pa×s	606.27	Joback Method
dvisc	0.0002208	Pa×s	652.18	Joback Method
dvisc	0.0001773	Pa×s	698.09	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2001298&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tf: Normal melting (fusion) point