

3-bromobenzophenone

Inchi:	InChI=1S/C13H9BrO/c14-12-8-4-7-11(9-12)13(15)10-5-2-1-3-6-10/h1-9H
InchiKey:	XNUMUNIJQMSNNN-UHFFFAOYSA-N
Formula:	C13H9BrO
SMILES:	O=C(c1ccccc1)c1cccc(Br)c1
Mol. weight [g/mol]:	261.11
CAS:	1016-77-9

Physical Properties

Property code	Value	Unit	Source
gf	159.17	kJ/mol	Joback Method
hf	63.69	kJ/mol	Joback Method
hfus	24.00	kJ/mol	Joback Method
hvap	62.93	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.680		Crippen Method
mcvol	165.580	ml/mol	McGowan Method
pc	3513.74	kPa	Joback Method
tb	675.21	K	Joback Method
tc	940.54	K	Joback Method
tf	350.15 ± 3.00	K	NIST Webbook
vc	0.616	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.17	J/mol×K	675.21	Joback Method
cpg	389.24	J/mol×K	719.43	Joback Method
cpg	401.10	J/mol×K	763.65	Joback Method
cpg	411.84	J/mol×K	807.88	Joback Method
cpg	421.56	J/mol×K	852.10	Joback Method
cpg	430.37	J/mol×K	896.32	Joback Method
cpg	438.36	J/mol×K	940.54	Joback Method
dvisc	0.0014329	Paxs	411.36	Joback Method
dvisc	0.0008791	Paxs	455.34	Joback Method

dvisc	0.0005878	Paxs	499.31	Joback Method
dvisc	0.0004195	Paxs	543.29	Joback Method
dvisc	0.0003149	Paxs	587.26	Joback Method
dvisc	0.0002460	Paxs	631.24	Joback Method
dvisc	0.0001985	Paxs	675.21	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C1016779&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
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

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