Benzoyl bromide

Inchi: InChI=1S/C7H5BrO/c8-7(9)6-4-2-1-3-5-6/h1-5H
InchiKey: AQIHMSVIAGNIDM-UHFFFAOYSA-N
Formula: C7H5BrO
SMILES: O=C(Br)c1ccccc1
Mol. weight [g/mol]: 185.02
CAS: 618-32-6

Physical Properties

Property code	Value	Unit	Source
gf	5.87	kJ/mol	Joback Method
hf	-48.50 ± 6.30	kJ/mol	NIST Webbook
hfl	-107.30 ± 0.71	kJ/mol	NIST Webbook
hfus	14.81	kJ/mol	Joback Method
hvap	58.60 ± 6.30	kJ/mol	NIST Webbook
ie	9.80	eV	NIST Webbook
ie	9.65	eV	NIST Webbook
ie	9.20	eV	NIST Webbook
log10ws	-2.64		Crippen Method
logp	2.222		Crippen Method
mcvol	104.800	ml/mol	McGowan Method
pc	4910.80	kPa	Joback Method
tb	491.50 ± 0.50	K	NIST Webbook
tb	491.70	K	NIST Webbook
tc	749.47	K	Joback Method
tf	249.00	K	NIST Webbook
vc	0.388	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	184.89	J/mol×K	506.27	Joback Method
cpg	194.53	J/mol×K	546.80	Joback Method
cpg	203.39	J/mol×K	587.34	Joback Method
cpg	211.50	J/mol×K	627.87	Joback Method

cpg	218.93	J/mol×K	668.40	Joback Method
cpg	225.71	J/mol×K	708.94	Joback Method
cpg	231.91	J/mol×K	749.47	Joback Method
dvisc	0.0026455	Pa×s	304.80	Joback Method
dvisc	0.0016055	Pa×s	338.38	Joback Method
dvisc	0.0010663	Pa×s	371.96	Joback Method
dvisc	0.0007579	Pa×s	405.53	Joback Method
dvisc	0.0005675	Pa×s	439.11	Joback Method
dvisc	0.0004428	Pa×s	472.69	Joback Method
dvisc	0.0003571	Pa×s	506.27	Joback Method
hvapt	52.30	kJ/mol	406.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	322.00 ± 1.00	K	0.01	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.57483e+01
Coeff. B	-5.10834e+03
Coeff. C	-3.26770e+01
Temperature range (K), min.	363.09
Temperature range (K), max.	522.13

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C618326&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1695.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume