Benzene, 1-bromo-4-(1,1-dimethylethyl)-

Other names:	1-Bromo-4-(1,1-dimethylethyl)benzene
	1-Bromo-4-t-butylbenzene
	1-Bromo-4-tert-butylbenzene
	1-tert-Butyl-4-Bromobenzene
	4-Bromo-t-butylbenzene
	4-Bromo-tert-butylbenzene
	4-t-Butylbromobenzene
	4-tert-Butyl-1-bromobenzene
	4-tert-Butylbromobenzene
	4-tert-Butylphenyl Bromide
	Benzene, 1-bromo-4-tert-butyl-
	NSC 43038
	p-Bromo-t-butylbenzene
	p-Bromo-tert-butylbenzene
	p-tert-Butylbromobenzene
Inchi:	InChI=1S/C10H13Br/c1-10(2,3)8-4-6-9(11)7-5-8/h4-7H,1-3H3
InchiKey:	XHCAGOVGSDHHNP-UHFFFAOYSA-N
Formula:	C10H13Br
SMILES:	CC(C)(C)c1ccc(Br)cc1
Mol. weight [g/mol]:	213.11
CAS:	3972-65-4

Physical Properties

Property code	Value	Unit	Source
gf	153.26	kJ/mol	Joback Method
hf	-7.09	kJ/mol	Joback Method
hfus	13.18	kJ/mol	Joback Method
hvap	45.93	kJ/mol	Joback Method
ie	8.48	eV	NIST Webbook
ie	8.68	eV	NIST Webbook
ie	8.50 ± 0.02	eV	NIST Webbook
log10ws	-3.95		Crippen Method
logp	3.747		Crippen Method
mcvol	145.500	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	504.00 ± 5.00	K	NIST Webbook
tc	759.79	K	Joback Method

tf	303.62	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.75	J/mol×K	522.79	Joback Method
cpg	316.73	J/mol×K	562.29	Joback Method
cpg	330.58	J/mol×K	601.79	Joback Method
cpg	343.36	J/mol×K	641.29	Joback Method
cpg	355.16	J/mol×K	680.79	Joback Method
cpg	366.06	J/mol×K	720.29	Joback Method
cpg	376.13	J/mol×K	759.79	Joback Method
dvisc	0.0026932	Pa×s	303.62	Joback Method
dvisc	0.0014454	Pa×s	340.15	Joback Method
dvisc	0.0008753	Pa×s	376.68	Joback Method
dvisc	0.0005792	Pa×s	413.20	Joback Method
dvisc	0.0004098	Pa×s	449.73	Joback Method
dvisc	0.0003055	Pa×s	486.26	Joback Method
dvisc	0.0002372	Pa×s	522.79	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	353.70	K	0.30	NIST Webbook
tbrp	376.20	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42272e+01
Coeff. B	-4.06027e+03
Coeff. C	-8.14430e+01

Temperature range (K), min.	372.72
Temperature range (K), max.	536.85

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3972654&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

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
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