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

Other names:	1-Bromo-4-isopropylbenzene
	2-(4-Bromophenyl)propane
	2-(p-Bromophenyl)propane
	4-Bromocumene
	4-Bromoisopropylbenzene
	4-Isopropylbromobenzene
	Cumene, p-bromo-
	p-Bromocumene
	p-Bromoisopropylbenzene
Inchi:	InChI=1S/C9H11Br/c1-7(2)8-3-5-9(10)6-4-8/h3-7H,1-2H3
InchiKey:	MOZHUOIQYVYEPN-UHFFFAOYSA-N
Formula:	C9H11Br
SMILES:	CC(C)c1ccc(Br)cc1
Mol. weight [g/mol]:	199.09
CAS:	586-61-8

Physical Properties

Property code	Value	Unit	Source
gf	139.56	kJ/mol	Joback Method
hf	17.02	kJ/mol	Joback Method
hfus	14.48	kJ/mol	Joback Method
hvap	44.61	kJ/mol	Joback Method
log10ws	-3.82		Crippen Method
logp	3.572		Crippen Method
mcvol	131.410	ml/mol	McGowan Method
pc	3505.43	kPa	Joback Method
tb	491.90	K	NIST Webbook
tb	491.92 ± 0.30	K	NIST Webbook
tc	733.98	K	Joback Method
tf	250.80 ± 0.02	K	NIST Webbook
tf	250.69 ± 0.05	K	NIST Webbook
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.04	J/mol×K	695.44	Joback Method
cpg	302.99	J/mol×K	656.89	Joback Method
cpg	292.20	J/mol×K	618.34	Joback Method
cpg	280.63	J/mol×K	579.79	Joback Method
cpg	268.23	J/mol×K	541.25	Joback Method
cpg	254.97	J/mol×K	502.70	Joback Method
cpg	322.39	J/mol×K	733.98	Joback Method
dvisc	0.0028478	Pa×s	274.93	Joback Method
dvisc	0.0002557	Pa×s	502.70	Joback Method
dvisc	0.0003242	Pa×s	464.74	Joback Method
dvisc	0.0004290	Pa×s	426.78	Joback Method
dvisc	0.0005995	Pa×s	388.81	Joback Method
dvisc	0.0009006	Pa×s	350.85	Joback Method
dvisc	0.0014935	Pa×s	312.89	Joback Method
hvapt	51.10	kJ/mol	427.50	NIST Webbook
hvapt	50.40	kJ/mol	458.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	370.70	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.41417e+01
Coeff. B	-3.94280e+03
Coeff. C	-7.78840e+01
Temperature range (K), min.	362.48
Temperature range (K), max.	524.40

Sources

Crippen Method:	https://www.chemeo.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=C586618&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

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
hvapt:	Enthalpy of vaporization at a given temperature
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

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