Benzene, 1-bromo-2-(1-methylethyl)-

Other names:	Cumene, o-bromo-
	o-Bromocumene
	o-Isopropylphenyl bromide
	1-Bromo-2-isopropylbenzene
	2-Bromoisopropylbenzene
	2-Isopropylbromobenzene
Inchi:	InChI=1S/C9H11Br/c1-7(2)8-5-3-4-6-9(8)10/h3-7H,1-2H3
InchiKey:	LECYCYNAEJDSIL-UHFFFAOYSA-N
Formula:	C9H11Br
SMILES:	CC(C)c1ccccc1Br
Mol. weight [g/mol]:	199.09
CAS:	7073-94-1

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	483.47 ± 0.30	K	NIST Webbook
tc	733.98	K	Joback Method
tf	214.25 ± 0.05	K	NIST Webbook
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.97	J/mol×K	502.70	Joback Method
cpg	268.23	J/mol×K	541.25	Joback Method
cpg	280.63	J/mol×K	579.79	Joback Method

cpg	292.20	J/mol×K	618.34	Joback Method
cpg	302.99	J/mol×K	656.89	Joback Method
cpg	313.04	J/mol×K	695.44	Joback Method
cpg	322.39	J/mol×K	733.98	Joback Method
dvisc	0.0014935	Pa×s	312.89	Joback Method
dvisc	0.0028478	Pa×s	274.93	Joback Method
dvisc	0.0009006	Pa×s	350.85	Joback Method
dvisc	0.0005995	Pa×s	388.81	Joback Method
dvisc	0.0004290	Pa×s	426.78	Joback Method
dvisc	0.0003242	Pa×s	464.74	Joback Method
dvisc	0.0002557	Pa×s	502.70	Joback Method
hvapt	48.40	kJ/mol	444.00	NIST Webbook
hvapt	49.80	kJ/mol	453.00	NIST Webbook

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=C7073941&Units=SI
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume