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

Other names:	Cumene, «beta»-bromo- «beta»-Bromoisopropylbenzene 1-Bromo-2-phenylpropane 2-Phenylpropyl bromide «beta»-Bromocumene
Inchi:	InChI=1S/C9H11Br/c1-8(7-10)9-5-3-2-4-6-9/h2-6,8H,7H2,1H3
InchiKey:	XJWVCWQKZQENDS-UHFFFAOYSA-N
Formula:	C9H11Br
SMILES:	CC(CBr)c1ccccc1
Mol. weight [g/mol]:	199.09
CAS:	1459-00-3

Physical Properties

Property code	Value	Unit	Source
gf	149.19	kJ/mol	Joback Method
hf	28.49	kJ/mol	Joback Method
hfus	14.87	kJ/mol	Joback Method
hvap	43.95	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	3.185		Crippen Method
mcvol	131.410	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	497.72	K	Joback Method
tc	727.72	K	Joback Method
tf	262.41	K	Joback Method
vc	0.487	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.95	J/mol×K	497.72	Joback Method
cpg	268.65	J/mol×K	536.05	Joback Method
cpg	281.41	J/mol×K	574.39	Joback Method
cpg	293.27	J/mol×K	612.72	Joback Method

cpg	304.28	J/mol×K	651.05	Joback Method
cpg	314.51	J/mol×K	689.39	Joback Method
cpg	323.99	J/mol×K	727.72	Joback Method
dvisc	0.0040622	Pa×s	262.41	Joback Method
dvisc	0.0019186	Pa×s	301.63	Joback Method
dvisc	0.0010769	Pa×s	340.85	Joback Method
dvisc	0.0006810	Pa×s	380.07	Joback Method
dvisc	0.0004692	Pa×s	419.28	Joback Method
dvisc	0.0003445	Pa×s	458.50	Joback Method
dvisc	0.0002656	Pa×s	497.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1459003&Units=SI
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
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