Cyclohexane, 1-bromo-4-methyl-

Other names:	p-Methylcyclohexyl bromide
	4-Methylcyclohexyl bromide
	4-Methylcyclohexyl bromide cis+trans
	1-bromo-4-methylcyclohexane
Inchi:	InChI=1S/C7H13Br/c1-6-2-4-7(8)5-3-6/h6-7H,2-5H2,1H3
InchiKey:	RLOHLPHAOHGRNM-UHFFFAOYSA-N
Formula:	C7H13Br
SMILES:	CC1CCC(Br)CC1
Mol. weight [g/mol]:	177.08
CAS:	6294-40-2

Physical Properties

Property code	Value	Unit	Source
gf	39.12	kJ/mol	Joback Method
hf	-127.50	kJ/mol	Joback Method
hfus	12.08	kJ/mol	Joback Method
hvap	37.73	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.960		Crippen Method
mcvol	116.130	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
tb	440.60	K	Joback Method
tc	663.39	K	Joback Method
tf	231.59	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.04	J/mol×K	440.60	Joback Method
cpg	234.42	J/mol×K	477.73	Joback Method
cpg	249.90	J/mol×K	514.86	Joback Method
cpg	264.49	J/mol×K	552.00	Joback Method
cpg	278.24	J/mol×K	589.13	Joback Method

cpg	291.16	J/mol×K	626.26	Joback Method
cpg	303.28	J/mol×K	663.39	Joback Method
dvisc	0.0037384	Pa×s	231.59	Joback Method
dvisc	0.0019742	Pa×s	266.43	Joback Method
dvisc	0.0012085	Pa×s	301.26	Joback Method
dvisc	0.0008189	Pa×s	336.09	Joback Method
dvisc	0.0005971	Pa×s	370.93	Joback Method
dvisc	0.0004596	Pa×s	405.76	Joback Method
dvisc	0.0003687	Pa×s	440.60	Joback Method

Sources

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=C6294402&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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