Cyclohexene, 1-bromo-4-methyl

Inchi: InChI=1S/C7H11Br/c1-6-2-4-7(8)5-3-6/h4,6H,2-3,5H2,1H3
InchiKey: LIUFYLLBQSSKQS-UHFFFAOYSA-N
Formula: C7H11Br
SMILES: CC1CC=C(Br)CC1
Mol. weight [g/mol]: 175.07

Physical Properties

Property code	Value	Unit	Source
gf	67.16	kJ/mol	Joback Method
hf	-60.85	kJ/mol	Joback Method
hfus	11.84	kJ/mol	Joback Method
hvap	38.99	kJ/mol	Joback Method
log10ws	-3.19		Crippen Method
logp	3.085		Crippen Method
mcvol	111.830	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
rinpol	1036.00		NIST Webbook
rinpol	1036.00		NIST Webbook
rinpol	1040.00		NIST Webbook
rinpol	1036.00		NIST Webbook
ripol	1361.00		NIST Webbook
ripol	1361.00		NIST Webbook
tb	449.41	K	Joback Method
tc	676.42	K	Joback Method
tf	249.11	K	Joback Method
vc	0.408	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.76	J/mol×K	449.41	Joback Method
cpg	217.90	J/mol×K	487.25	Joback Method
cpg	231.21	J/mol×K	525.08	Joback Method
cpg	243.72	J/mol×K	562.92	Joback Method

cpg	255.46	J/mol×K	600.75	Joback Method
cpg	266.46	J/mol×K	638.59	Joback Method
cpg	276.75	J/mol×K	676.42	Joback Method
dvisc	0.0030799	Pa×s	249.11	Joback Method
dvisc	0.0017171	Pa×s	282.49	Joback Method
dvisc	0.0010832	Pa×s	315.88	Joback Method
dvisc	0.0007462	Pa×s	349.26	Joback Method
dvisc	0.0005486	Pa×s	382.64	Joback Method
dvisc	0.0004237	Pa×s	416.03	Joback Method
dvisc	0.0003401	Pa×s	449.41	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R25441&Units=SI

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
rinpol: Non-polar retention indices
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume