1,4-Cyclohexadiene, 1-bromo

Inchi: InChI=1S/C6H7Br/c7-6-4-2-1-3-5-6/h1-2,5H,3-4H2
InchiKey: HBPTXOABIPHZOS-UHFFFAOYSA-N
Formula: C6H7Br
SMILES: BrC1=CCC=CC1
Mol. weight [g/mol]: 159.02

Physical Properties

Property code	Value	Unit	Source
gf	96.41	kJ/mol	Joback Method
hf	37.91	kJ/mol	Joback Method
hfus	9.40	kJ/mol	Joback Method
hvap	37.37	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	2.615		Crippen Method
mcvol	93.440	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
rinpol	1021.00		NIST Webbook
tb	430.36	K	Joback Method
tc	663.66	K	Joback Method
tf	242.84	K	Joback Method
vc	0.340	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.28	J/mol×K	430.36	Joback Method
cpg	197.06	J/mol×K	624.78	Joback Method
cpg	188.88	J/mol×K	585.90	Joback Method
cpg	180.06	J/mol×K	547.01	Joback Method
cpg	170.54	J/mol×K	508.13	Joback Method
cpg	160.29	J/mol×K	469.24	Joback Method
cpg	204.62	J/mol×K	663.66	Joback Method
dvisc	0.0003474	Pa×s	430.36	Joback Method
dvisc	0.0004393	Pa×s	399.11	Joback Method

dvisc	0.0005781	Pa×s	367.85	Joback Method
dvisc	0.0008004	Pa×s	336.60	Joback Method
dvisc	0.0011846	Pa×s	305.35	Joback Method
dvisc	0.0019173	Pa×s	274.09	Joback Method
dvisc	0.0035125	Pa×s	242.84	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R25348&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume