1,4-Cyclohexadiene, 6-bromo

Inchi: InChI=1S/C6H7Br/c7-6-4-2-1-3-5-6/h2-6H,1H2
InchiKey: KZXYAVCLVOWUHC-UHFFFAOYSA-N
Formula: C6H7Br
SMILES: BrC1C=CCC=C1
Mol. weight [g/mol]: 159.02

Physical Properties

Property code	Value	Unit	Source
gf	98.33	kJ/mol	Joback Method
hf	29.04	kJ/mol	Joback Method
hfus	10.86	kJ/mol	Joback Method
hvap	36.40	kJ/mol	Joback Method
log10ws	-2.48		Crippen Method
logp	2.266		Crippen Method
mcvol	93.440	ml/mol	McGowan Method
pc	4769.39	kPa	Joback Method
rinpol	1020.00		NIST Webbook
tb	420.71	K	Joback Method
tc	652.02	K	Joback Method
tf	226.08	K	Joback Method
vc	0.339	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.64	J/mol×K	420.71	Joback Method
cpg	161.56	J/mol×K	459.26	Joback Method
cpg	172.67	J/mol×K	497.81	Joback Method
cpg	183.00	J/mol×K	536.36	Joback Method
cpg	192.59	J/mol×K	574.91	Joback Method
cpg	201.48	J/mol×K	613.47	Joback Method
cpg	209.71	J/mol×K	652.02	Joback Method
dvisc	0.0033740	Pa×s	226.08	Joback Method
dvisc	0.0018395	Pa×s	258.52	Joback Method

dvisc	0.0011482	Pa×s	290.96	Joback Method
dvisc	0.0007877	Pa×s	323.39	Joback Method
dvisc	0.0005789	Pa×s	355.83	Joback Method
dvisc	0.0004478	Pa×s	388.27	Joback Method
dvisc	0.0003605	Pa×s	420.71	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R25384&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