

1,3-Cyclohexadiene, 6-bromo

Inchi:	InChI=1S/C6H7Br/c7-6-4-2-1-3-5-6/h1-4,6H,5H2
InchiKey:	ZNHUWWLVGFLEMW-UHFFFAOYSA-N
Formula:	C6H7Br
SMILES:	BrC1C=CC=CC1
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	972.00		NIST Webbook
tb	420.71	K	Joback Method
tc	652.02	K	Joback Method
tf	226.08	K	Joback Method
vc	0.339	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0011482	Paxs	290.96	Joback Method
dvisc	0.0007877	Paxs	323.39	Joback Method
dvisc	0.0005789	Paxs	355.83	Joback Method
dvisc	0.0004478	Paxs	388.27	Joback Method
dvisc	0.0003605	Paxs	420.71	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=R25302&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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