

1,3-Cyclohexadiene, 2-bromo

Inchi:	InChI=1S/C6H7Br/c7-6-4-2-1-3-5-6/h2,4-5H,1,3H2
InchiKey:	IYBFVRUXEKUNNQ-UHFFFAOYSA-N
Formula:	C6H7Br
SMILES:	BrC1=CCCC=C1
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	980.00		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/molxK	430.36	Joback Method
cpg	160.29	J/molxK	469.24	Joback Method
cpg	170.54	J/molxK	508.13	Joback Method
cpg	180.06	J/molxK	547.01	Joback Method
cpg	188.88	J/molxK	585.90	Joback Method
cpg	197.06	J/molxK	624.78	Joback Method
cpg	204.62	J/molxK	663.66	Joback Method
dvisc	0.0035125	Paxs	242.84	Joback Method
dvisc	0.0019173	Paxs	274.09	Joback Method

dvisc	0.0011846	Paxs	305.35	Joback Method
dvisc	0.0008004	Paxs	336.60	Joback Method
dvisc	0.0005781	Paxs	367.85	Joback Method
dvisc	0.0004393	Paxs	399.11	Joback Method
dvisc	0.0003474	Paxs	430.36	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=R25259&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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