

Cyclohexene, 1,6-dibromo

Inchi:	InChI=1S/C6H8Br2/c7-5-3-1-2-4-6(5)8/h3,6H,1-2,4H2
InchiKey:	GOMHXBPKIHKYIA-UHFFFAOYSA-N
Formula:	C6H8Br2
SMILES:	BrC1=CCCCC1Br
Mol. weight [g/mol]:	239.94

Physical Properties

Property code	Value	Unit	Source
gf	73.06	kJ/mol	Joback Method
hf	-13.88	kJ/mol	Joback Method
hfus	14.53	kJ/mol	Joback Method
hvap	43.20	kJ/mol	Joback Method
log10ws	-3.55		Crippen Method
logp	3.213		Crippen Method
mcvol	115.240	ml/mol	McGowan Method
pc	4890.21	kPa	Joback Method
rinpol	1282.00		NIST Webbook
rinpol	1282.00		NIST Webbook
rinpol	1288.00		NIST Webbook
rinpol	1288.00		NIST Webbook
tb	492.69	K	Joback Method
tc	742.26	K	Joback Method
tf	297.64	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.50	J/molxK	492.69	Joback Method
cpg	211.60	J/molxK	534.29	Joback Method
cpg	222.81	J/molxK	575.88	Joback Method
cpg	233.17	J/molxK	617.48	Joback Method
cpg	242.74	J/molxK	659.07	Joback Method
cpg	251.57	J/molxK	700.67	Joback Method

cpg	259.70	J/mol×K	742.26	Joback Method
dvisc	0.0025998	Paxs	297.64	Joback Method
dvisc	0.0016241	Paxs	330.15	Joback Method
dvisc	0.0011038	Paxs	362.66	Joback Method
dvisc	0.0007994	Paxs	395.16	Joback Method
dvisc	0.0006081	Paxs	427.67	Joback Method
dvisc	0.0004808	Paxs	460.18	Joback Method
dvisc	0.0003921	Paxs	492.69	Joback Method

Sources

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=R25437&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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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