

Cyclohexane, 1,4-dibromo-

Other names:	1,4-Dibromocyclohexane
Inchi:	InChI=1S/C6H10Br2/c7-5-1-2-6(8)4-3-5/h5-6H,1-4H2
InchiKey:	OALGWDQLKYPDRK-UHFFFAOYSA-N
Formula:	C6H10Br2
SMILES:	BrC1CCC(Br)CC1
Mol. weight [g/mol]:	241.95
CAS:	35076-92-7

Physical Properties

Property code	Value	Unit	Source
gf	45.02	kJ/mol	Joback Method
hf	-80.53	kJ/mol	Joback Method
hfus	14.77	kJ/mol	Joback Method
hvap	41.94	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	3.087		Crippen Method
mcvol	119.540	ml/mol	McGowan Method
pc	4540.80	kPa	Joback Method
tb	483.88	K	Joback Method
tc	729.25	K	Joback Method
tf	278.85 ± 0.50	K	NIST Webbook
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	217.19	J/mol×K	483.88	Joback Method
cpg	280.16	J/mol×K	688.35	Joback Method
cpg	269.38	J/mol×K	647.46	Joback Method
cpg	257.74	J/mol×K	606.56	Joback Method
cpg	245.19	J/mol×K	565.67	Joback Method
cpg	231.69	J/mol×K	524.77	Joback Method
cpg	290.13	J/mol×K	729.25	Joback Method
dvisc	0.0004316	Pa×s	483.88	Joback Method

dvisc	0.0005303	Pa×s	449.92	Joback Method
dvisc	0.0006741	Pa×s	415.96	Joback Method
dvisc	0.0008941	Pa×s	382.00	Joback Method
dvisc	0.0012531	Pa×s	348.04	Joback Method
dvisc	0.0018892	Pa×s	314.08	Joback Method
dvisc	0.0031464	Pa×s	280.12	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=C35076927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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