Cyclohexane, 1,2-dibromo-

Other names: 1,2-Dibromocyclohexane
Inchi: InChI=1S/C6H10Br2/c7-5-3-1-2-4-6(5)8/h5-6H,1-4H2
InchiKey: CZNHKZKWKJNOTE-UHFFFAOYSA-N
Formula: C6H10Br2
SMILES: BrC1CCCCC1Br
Mol. weight [g/mol]: 241.95
CAS: 5401-62-7

Physical Properties

Property code	Value	Unit	Source
chl	-3629.80 ± 2.50	kJ/mol	NIST Webbook
gf	45.02	kJ/mol	Joback Method
hf	-109.90 ± 2.90	kJ/mol	NIST Webbook
hfl	-160.50 ± 2.50	kJ/mol	NIST Webbook
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	280.12	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	290.13	J/mol×K	729.25	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	217.19	J/mol×K	483.88	Joback Method
dvisc	0.0031464	Pa×s	280.12	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
hvapt	50.50	kJ/mol	300.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.66518e+01
Coeff. B	-6.00321e+03
Coeff. C	1.18188e-04
Coeff. D	-2.67308e-10
Temperature range (K), min.	273.15
Temperature range (K), max.	332.15

Sources

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1759
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
KDB: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1759
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5401627&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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