Cyclohexane,1,2-dibromo-,trans-

Other names: .+/-.-trans-1,2-Dibromocyclohexane
trans-1,2-Dibromocyclohexane
Inchi: InChI=1S/C6H10Br2/c7-5-3-1-2-4-6(5)8/h5-6H,1-4H2/t5-,6-/m0/s1
InchiKey: CZNHKZKWKJNOTE-WDSKDSINSA-N
Formula: C6H10Br2
SMILES: BrC1CCCCC1Br
Mol. weight [g/mol]: 241.95
CAS: 7429-37-0

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	50.50	kJ/mol	NIST Webbook
ie	10.06 ± 0.01	eV	NIST Webbook
ie	10.02 ± 0.02	eV	NIST Webbook
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	217.19	J/mol×K	483.88	Joback Method
cpg	231.69	J/mol×K	524.77	Joback Method
cpg	245.19	J/mol×K	565.67	Joback Method
cpg	257.74	J/mol×K	606.56	Joback Method
cpg	269.38	J/mol×K	647.46	Joback Method

cpg	280.16	J/mol×K	688.35	Joback Method
cpg	290.13	J/mol×K	729.25	Joback Method
dvisc	0.0031464	Pa×s	280.12	Joback Method
dvisc	0.0018892	Pa×s	314.08	Joback Method
dvisc	0.0012531	Pa×s	348.04	Joback Method
dvisc	0.0008941	Pa×s	382.00	Joback Method
dvisc	0.0006741	Pa×s	415.96	Joback Method
dvisc	0.0005303	Pa×s	449.92	Joback Method
dvisc	0.0004316	Pa×s	483.88	Joback Method
hvapt	53.30	kJ/mol	383.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.20	K	13.30	NIST Webbook
tbrp	374.00 ± 2.00	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.96449e+01
Coeff. B	-7.65778e+03
Coeff. C	3.17290e+01
Temperature range (K), min.	363.87
Temperature range (K), max.	502.53

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=C7429370&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume