1,2-DIBROMOTETRACHLOROETHANE

Other names:	1,2-Dibromo-1,1,2,2-tetrachloroethane
	Dbtce
	Ethane, 1,2-dibromo-tetrachloro-
	sym-Dibromotetrachloroethane
Inchi:	InChI=1S/C2Br2Cl4/c3-1(5,6)2(4,7)8
InchiKey:	WJUKOGPNGRUXMG-UHFFFAOYSA-N
Formula:	C2Br2Cl4
SMILES:	ClC(Cl)(Br)C(Cl)(Cl)Br
Mol. weight [g/mol]:	325.64
CAS:	630-25-1

Physical Properties

Property code	Value	Unit	Source
af	0.3106		Cheméo Relay (1.0)
hf	-66.73	kJ/mol	Cheméo Relay (1.0)
hfus	13.47	kJ/mol	Joback Method
hvap	51.78	kJ/mol	Cheméo Relay (1.0)
ie	10.60	eV	Cheméo Relay (1.0)
logp	4.039		Crippen Method
mcvol	123.000	ml/mol	McGowan Method
pc	5235.81	kPa	Joback Method
tb	492.06	K	Cheméo Relay (1.0)
tc	723.86	K	Cheméo Relay (1.0)
tf	423.37	K	Cheméo Relay (1.0)
vc	0.447	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.75	J/mol×K	793.32	Joback Method
cpg	173.83	J/mol×K	702.46	Joback Method
cpg	165.68	J/mol×K	520.74	Joback Method
cpg	168.87	J/mol×K	566.17	Joback Method
cpg	171.20	J/mol×K	611.60	Joback Method

cpg	172.80	J/mol×K	657.03	Joback Method
cpg	174.43	J/mol×K	747.89	Joback Method
dvisc	0.0028387	Pa×s	356.42	Joback Method
dvisc	0.0018148	Pa×s	383.81	Joback Method
dvisc	0.0012314	Pa×s	411.19	Joback Method
dvisc	0.0008771	Pa×s	438.58	Joback Method
dvisc	0.0006501	Pa×s	465.97	Joback Method
dvisc	0.0004981	Pa×s	493.35	Joback Method
dvisc	0.0003925	Pa×s	520.74	Joback Method
hsubt	52.50	kJ/mol	418.00	NIST Webbook
hsubt	56.70	kJ/mol	373.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.68204e+01
Coeff. B	-6.30908e+03
Temperature range (K), min.	381.61
Temperature range (K), max.	548.19

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C630251&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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