Ethane, 1,1,2,2-tetrabromo-

Other names:	1,1,2,2-Tetrabromaethan
	1,1,2,2-Tetrabromoetano
	1,1,2,2-Tetrabromoethane
	1,1,2,2-Tetrabromoethylene
	1,1,2,2-Tetrabroomethaan
	ACETYLENE TETRABROMIDE
	Acetylene tetrabomide
	Muthmann's liquid
	NSC 406889
	TBE
	TETRABROMOETHANE
	Tetrabromoacetylene
	s-Tetrabromoethane
	sym-Tetrabromoethane
Inchi:	InChI=1S/C2H2Br4/c3-1(4)2(5)6/h1-2H
InchiKey:	QXSZNDIIPUOQMB-UHFFFAOYSA-N
Formula:	C2H2Br4
SMILES:	BrC(Br)C(Br)Br
Mol. weight [g/mol]:	345.65
CAS:	79-27-6

Physical Properties

Property code	Value	Unit	Source
gf	18.36	kJ/mol	Joback Method
hf	10.15	kJ/mol	Joback Method
hfus	15.03	kJ/mol	Joback Method
hvap	45.01	kJ/mol	Joback Method
log10ws	-2.72		Aqueous Solubility Prediction Method
logp	3.218		Crippen Method
mcvol	109.040	ml/mol	McGowan Method
pc	8000.49	kPa	Joback Method
rinpol	1245.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1265.00		NIST Webbook
rinpol	1226.00		NIST Webbook
rinpol	1226.00		NIST Webbook

rinpol	1269.00		NIST Webbook
tb	516.70	K	NIST Webbook
tb	407.15	K	KDB
tc	771.57	K	Joback Method
tf	272.20 ± 0.60	K	NIST Webbook
tf	273.15	K	KDB
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	148.67	J/mol×K	727.79	Joback Method
cpg	144.24	J/mol×K	640.24	Joback Method
cpg	141.52	J/mol×K	596.47	Joback Method
cpg	138.38	J/mol×K	552.69	Joback Method
cpg	134.73	J/mol×K	508.92	Joback Method
cpg	146.60	J/mol×K	684.02	Joback Method
cpg	150.55	J/mol×K	771.57	Joback Method
cpl	165.70	J/mol×K	298.00	NIST Webbook
dvisc	0.0030131	Pa×s	321.50	Joback Method
dvisc	0.0004232	Pa×s	508.92	Joback Method
dvisc	0.0005275	Pa×s	477.68	Joback Method
dvisc	0.0006780	Pa×s	446.45	Joback Method
dvisc	0.0009049	Pa×s	415.21	Joback Method
dvisc	0.0012659	Pa×s	383.97	Joback Method
dvisc	0.0018795	Pa×s	352.74	Joback Method
hvapt	56.90	kJ/mol	493.00	NIST Webbook
rfi	1.62926		303.15	Densities, excess molar volumes, and refractive indices of 1,1,2,2-tetrabromoethane and 1-alkanols binary mixtures
rfi	1.63535		293.15	Excess molar volumes and viscosities of (1,1,2,2-tetrabromoethane + 1-alkanols) at T = (293.15 and 303.15) K

rfi	1.63535		293.15	Densities, excess molar volumes, and refractive indices of 1,1,2,2-tetrabromoethane and 1-alkanols binary mixtures

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	392.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54484e+01
Coeff. B	-4.67772e+03
Coeff. C	-8.47790e+01
Temperature range (K), min.	393.32
Temperature range (K), max.	546.23

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.90307e+02
Coeff. B	-1.58728e+04
Coeff. C	-2.52435e+01
Coeff. D	1.02136e-05
Temperature range (K), min.	273.15
Temperature range (K), max.	824.00

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1554.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79276&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Excess molar volumes and viscosities of (1,1,2,2-tetrabromoethane + 1-alkanols) at T = (298.15 and 303.15) K:	https://www.doi.org/10.1016/j.jct.2005.03.027
Densities, excess molar volumes, and refractive indices of 1,1,2,2-tetrabromoethane and 1-alkanols binary mixtures:	https://www.doi.org/10.1016/j.jct.2005.11.012
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1554

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rfi:	Refractive Index
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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