1,1,1,2-Tetrabromoethane

Other names: Ethane, 1,1,1,2-tetrabromo-
Inchi: InChI=1S/C2H2Br4/c3-1-2(4,5)6/h1H2
InchiKey: RVHSTXJKKZWWDQ-UHFFFAOYSA-N
Formula: C2H2Br4
SMILES: BrCC(Br)(Br)Br
Mol. weight [g/mol]: 345.65
CAS: 630-16-0

Physical Properties

Property code	Value	Unit	Source
gf	26.08	kJ/mol	Joback Method
hf	11.96	kJ/mol	Joback Method
hfus	14.66	kJ/mol	Joback Method
hvap	44.49	kJ/mol	Joback Method
log10ws	-3.49		Crippen Method
logp	3.220		Crippen Method
mcvol	109.040	ml/mol	McGowan Method
pc	8043.60	kPa	Joback Method
tb	506.57	K	Joback Method
tc	774.77	K	Joback Method
tf	353.92	K	Joback Method
vc	0.385	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	152.51	J/mol×K	774.77	Joback Method
cpg	138.19	J/mol×K	506.57	Joback Method
cpg	141.95	J/mol×K	551.27	Joback Method
cpg	145.01	J/mol×K	595.97	Joback Method
cpg	147.47	J/mol×K	640.67	Joback Method
cpg	149.46	J/mol×K	685.37	Joback Method
cpg	151.10	J/mol×K	730.07	Joback Method
dvisc	0.0004563	Pa×s	506.57	Joback Method

dvisc	0.0022584	Pa×s	353.92	Joback Method
dvisc	0.0015821	Pa×s	379.36	Joback Method
dvisc	0.0011590	Pa×s	404.80	Joback Method
dvisc	0.0008808	Pa×s	430.25	Joback Method
dvisc	0.0006903	Pa×s	455.69	Joback Method
dvisc	0.0005551	Pa×s	481.13	Joback Method
hvapt	61.50	kJ/mol	402.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72925e+01
Coeff. B	-5.30440e+03
Coeff. C	-8.65860e+01
Temperature range (K), min.	398.52
Temperature range (K), max.	529.32

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C630160&Units=SI

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

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
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