

Ethene, tetrabromo-

Other names:	Ethylene, tetrabromo- Tetrabromoethene Tetrabromoethylene
Inchi:	InChI=1S/C2Br4/c3-1(4)2(5)6
InchiKey:	OVR RJBSHBOXFQE-UHFFFAOYSA-N
Formula:	C2Br4
SMILES:	BrC(Br)=C(Br)Br
Mol. weight [g/mol]:	343.64
CAS:	79-28-7

Physical Properties

Property code	Value	Unit	Source
gf	86.36	kJ/mol	Joback Method
hf	118.35	kJ/mol	Joback Method
hfus	19.66	kJ/mol	Joback Method
hvap	45.90	kJ/mol	Joback Method
ie	9.11	eV	NIST Webbook
log10ws	-4.22		Crippen Method
logp	3.693		Crippen Method
mcvol	104.740	ml/mol	McGowan Method
pc	8701.83	kPa	Joback Method
tb	499.70	K	NIST Webbook
tc	787.85	K	Joback Method
tf	318.50	K	Joback Method
vc	0.378	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	121.14	J/mol×K	742.16	Joback Method
cpg	114.48	J/mol×K	513.72	Joback Method
cpg	116.61	J/mol×K	559.41	Joback Method
cpg	118.23	J/mol×K	605.10	Joback Method
cpg	119.45	J/mol×K	650.79	Joback Method

cpg	120.38	J/mol×K	696.47	Joback Method
cpg	121.84	J/mol×K	787.85	Joback Method
hsubt	44.20	kJ/mol	265.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	373.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	5.97876e+00
Coeff. B	-4.20540e+02
Coeff. C	-1.90579e+02
Temperature range (K), min.	264.47
Temperature range (K), max.	820.80

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C79287&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/ci990307I
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

Legend

cpg: Ideal gas heat capacity

gf:	Standard Gibbs free energy of formation
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
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

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