Ethene, tribromo-

Other names:	Ethylene, tribromo- Tribromoethylene 1,1,2-Tribromoethylene Tribromoethene
Inchi:	InChI=1S/C2HBr3/c3-1-2(4)5/h1H
InchiKey:	OZVJKTHTULCNHB-UHFFFAOYSA-N
Formula:	C2HBr3
SMILES:	BrC=C(Br)Br
Mol. weight [g/mol]:	264.74
CAS:	598-16-3

Physical Properties

Property code	Value	Unit	Source
gf	80.59	kJ/mol	Joback Method
hf	101.81	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	39.39	kJ/mol	Joback Method
ie	9.27	eV	NIST Webbook
ie	9.27 ± 0.01	eV	NIST Webbook
log10ws	-3.29		Crippen Method
logp	2.970		Crippen Method
mcvol	87.240	ml/mol	McGowan Method
pc	7614.31	kPa	Joback Method
rinpol	978.00		NIST Webbook
rinpol	961.00		NIST Webbook
rinpol	978.00		NIST Webbook
rinpol	978.00		NIST Webbook
tb	437.20	K	NIST Webbook
tc	697.23	K	Joback Method
tf	272.66	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	96.25	J/mol×K	447.68	Joback Method
cpg	99.38	J/mol×K	489.27	Joback Method
cpg	102.02	J/mol×K	530.86	Joback Method
cpg	104.23	J/mol×K	572.46	Joback Method
cpg	106.08	J/mol×K	614.05	Joback Method
cpg	107.64	J/mol×K	655.64	Joback Method
cpg	108.99	J/mol×K	697.23	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	348.20	K	2.00	NIST Webbook

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=C598163&Units=SI

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
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
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