

Ethene, 1,2-dibromo-, (E)-

Other names:	(E)-1,2-Dibromoethylene
Inchi:	InChI=1S/C2H2Br2/c3-1-2-4/h1-2H/b2-1+
InchiKey:	UWTUEMKLYAGTNQ-OWOJBTEDSA-N
Formula:	C2H2Br2
SMILES:	BrC=CB
Mol. weight [g/mol]:	185.84
CAS:	590-12-5

Physical Properties

Property code	Value	Unit	Source
gf	74.82	kJ/mol	Joback Method
hf	85.27	kJ/mol	Joback Method
hfus	11.71	kJ/mol	Joback Method
hvap	32.87	kJ/mol	Joback Method
ie	9.55	eV	NIST Webbook
ie	9.56	eV	NIST Webbook
ie	9.47 ± 0.01	eV	NIST Webbook
ie	9.55 ± 0.01	eV	NIST Webbook
ie	9.30 ± 0.02	eV	NIST Webbook
ie	9.46 ± 0.02	eV	NIST Webbook
ie	9.47	eV	NIST Webbook
log10ws	-2.37		Crippen Method
logp	2.247		Crippen Method
mcvol	69.740	ml/mol	McGowan Method
pc	6718.62	kPa	Joback Method
rinpol	756.00		NIST Webbook
rinpol	730.00		NIST Webbook
rinpol	744.00		NIST Webbook
rinpol	738.00		NIST Webbook
rinpol	756.00		NIST Webbook
ripol	1139.04		NIST Webbook
ripol	1157.92		NIST Webbook
ripol	1150.25		NIST Webbook
tb	381.64	K	Joback Method
tc	604.03	K	Joback Method
tf	226.82	K	Joback Method
vc	0.252	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.00	J/molxK	566.97	Joback Method
cpg	93.12	J/molxK	604.03	Joback Method
cpg	75.76	J/molxK	381.64	Joback Method
cpg	79.56	J/molxK	418.71	Joback Method
cpg	82.94	J/molxK	455.77	Joback Method
cpg	85.95	J/molxK	492.84	Joback Method
cpg	88.63	J/molxK	529.90	Joback Method
dvisc	0.0004097	Paxs	381.64	Joback Method
dvisc	0.0004997	Paxs	355.84	Joback Method
dvisc	0.0026536	Paxs	226.82	Joback Method
dvisc	0.0016579	Paxs	252.62	Joback Method
dvisc	0.0011301	Paxs	278.43	Joback Method
dvisc	0.0008221	Paxs	304.23	Joback Method
dvisc	0.0006286	Paxs	330.03	Joback Method
hvapt	42.90	kJ/mol	310.00	NIST Webbook
hvapt	35.20	kJ/mol	310.50	NIST Webbook

Sources

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=C590125&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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