Ethane, 1,2-diiodo-

Other names:	1,2-Diiodoethane
	CH2ICH2I
	Diiodoethane
	ETHYLENE IODIDE
Inchi:	InChI=1S/C2H4I2/c3-1-2-4/h1-2H2
InchiKey:	GBBZLMLLFVFKJM-UHFFFAOYSA-N
Formula:	C2H4I2
SMILES:	ICCI
Mol. weight [g/mol]:	281.86
CAS:	624-73-7

Physical Properties

Property code	Value	Unit	Source
af	0.2230		KDB
chs	-1368.00 ± 0.60	kJ/mol	NIST Webbook
gf	82.20	kJ/mol	Joback Method
hf	66.80 ± 1.70	kJ/mol	NIST Webbook
hf	73.30 ± 1.10	kJ/mol	NIST Webbook
hfs	9.30 ± 0.80	kJ/mol	NIST Webbook
hfus	9.75	kJ/mol	Joback Method
hsub	64.00 ± 0.70	kJ/mol	NIST Webbook
hvap	49.80	kJ/mol	NIST Webbook
ie	9.40	eV	NIST Webbook
ie	9.50 ± 0.02	eV	NIST Webbook
log10ws	-2.56		Crippen Method
logp	1.856		Crippen Method
mcvol	90.680	ml/mol	McGowan Method
pc	4730.00	kPa	KDB
rinpol	1002.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	1015.00		NIST Webbook
rinpol	1008.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1008.00		NIST Webbook
tb	473.20	K	KDB
tb	473.20	K	NIST Webbook
tc	749.90	K	KDB

tf	356.00	K	KDB
vc	0.324	m3/kmol	KDB
zc	0.2454120		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	123.98	J/mol×K	683.78	Joback Method
cpg	121.24	J/mol×K	641.73	Joback Method
cpg	118.26	J/mol×K	599.67	Joback Method
cpg	114.98	J/mol×K	557.61	Joback Method
cpg	111.38	J/mol×K	515.55	Joback Method
cpg	107.40	J/mol×K	473.50	Joback Method
cpg	103.01	J/mol×K	431.44	Joback Method
dvisc	0.0060296	Pa×s	228.42	Joback Method
dvisc	0.0004990	Pa×s	431.44	Joback Method
dvisc	0.0006334	Pa×s	397.60	Joback Method
dvisc	0.0008406	Pa×s	363.77	Joback Method
dvisc	0.0011822	Pa×s	329.93	Joback Method
dvisc	0.0017975	Pa×s	296.09	Joback Method
dvisc	0.0030448	Pa×s	262.26	Joback Method
hvapt	47.70	kJ/mol	448.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.22119e+01
Coeff. B	-2.46094e+03
Coeff. C	-1.49119e+02
Temperature range (K), min.	355.50
Temperature range (K), max.	505.75

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2

Coeff. A	8.57571e+01
Coeff. B	-9.24244e+03
Coeff. C	-1.01406e+01
Coeff. D	3.82987e-06
Temperature range (K), min.	371.15
Temperature range (K), max.	749.91

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1576.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C624737&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1576
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume
zc:	Critical Compressibility