

1,1-diiodoethane

Inchi:	InChI=1S/C2H4I2/c1-2(3)4/h2H,1H3
InchiKey:	JNVXRQOSRUDXDY-UHFFFAOYSA-N
Formula:	C2H4I2
SMILES:	CC(I)I
Mol. weight [g/mol]:	281.86
CAS:	594-02-5

Physical Properties

Property code	Value	Unit	Source
gf	79.76	kJ/mol	Joback Method
hf	63.85	kJ/mol	Joback Method
hfus	6.23	kJ/mol	Joback Method
hvap	38.40	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.202		Crippen Method
mcvol	90.680	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	431.00	K	Joback Method
tc	690.03	K	Joback Method
tf	213.42	K	Joback Method
vc	0.318	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	103.20	J/mol×K	431.00	Joback Method
cpg	107.82	J/mol×K	474.17	Joback Method
cpg	111.99	J/mol×K	517.34	Joback Method
cpg	115.76	J/mol×K	560.51	Joback Method
cpg	119.17	J/mol×K	603.69	Joback Method
cpg	122.26	J/mol×K	646.86	Joback Method
cpg	125.09	J/mol×K	690.03	Joback Method
dvisc	0.0091347	Pa×s	213.42	Joback Method
dvisc	0.0039086	Pa×s	249.68	Joback Method

dvisc	0.0020742	Pa×s	285.95	Joback Method
dvisc	0.0012695	Pa×s	322.21	Joback Method
dvisc	0.0008581	Pa×s	358.47	Joback Method
dvisc	0.0006233	Pa×s	394.74	Joback Method
dvisc	0.0004778	Pa×s	431.00	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.70	K	1.60	NIST Webbook

Sources

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=C594025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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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