Propane, 1,3-diiodo-

Other names: 1,3-Diiodopropane
Trimethylene diiodide
Inchi: InChI=1S/C3H6I2/c4-2-1-3-5/h1-3H2
InchiKey: AAAXMNYUNVCMCJ-UHFFFAOYSA-N
Formula: C3H6I2
SMILES: ICCCI
Mol. weight [g/mol]: 295.89
CAS: 627-31-6

Physical Properties

Property code	Value	Unit	Source
chl	-2029.10 ± 1.00	kJ/mol	NIST Webbook
gf	90.62	kJ/mol	Joback Method
hf	44.00 ± 2.00	kJ/mol	NIST Webbook
hf	45.20 ± 1.50	kJ/mol	NIST Webbook
hfl	-8.90 ± 1.40	kJ/mol	NIST Webbook
hfus	12.34	kJ/mol	Joback Method
hvap	54.10 ± 0.60	kJ/mol	NIST Webbook
hvap	54.10	kJ/mol	NIST Webbook
log10ws	-2.97		Crippen Method
logp	2.247		Crippen Method
mcvol	104.770	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	454.32	K	Joback Method
tc	702.31	K	Joback Method
tf	239.69	K	Joback Method
vc	0.380	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.59	J/mol×K	454.32	Joback Method
cpg	143.81	J/mol×K	495.65	Joback Method
cpg	149.52	J/mol×K	536.98	Joback Method

cpg	154.77	J/mol×K	578.31	Joback Method
cpg	159.61	J/mol×K	619.64	Joback Method
cpg	164.08	J/mol×K	660.98	Joback Method
cpg	168.22	J/mol×K	702.31	Joback Method
cpl	169.20	J/mol×K	298.15	NIST Webbook
dvisc	0.0059900	Pa×s	239.69	Joback Method
dvisc	0.0029557	Pa×s	275.46	Joback Method
dvisc	0.0017156	Pa×s	311.23	Joback Method
dvisc	0.0011140	Pa×s	347.00	Joback Method
dvisc	0.0007841	Pa×s	382.78	Joback Method
dvisc	0.0005861	Pa×s	418.55	Joback Method
dvisc	0.0004586	Pa×s	454.32	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	385.20	K	4.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.18314e+01
Coeff. B	-2.76877e+03
Coeff. C	-1.28620e+02
Temperature range (K), min.	368.47
Temperature range (K), max.	553.28

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C627316&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/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
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