

Benzene, 1,3-diiodo-

Other names:	1,3-Diiodobenzene Benzene, m-diiodo- m-Diiodobenzene
Inchi:	InChI=1S/C6H4I2/c7-5-2-1-3-6(8)4-5/h1-4H
InchiKey:	SFPQFQUXAJOWNF-UHFFFAOYSA-N
Formula:	C6H4I2
SMILES:	Ic1cccc(I)c1
Mol. weight [g/mol]:	329.90
CAS:	626-00-6

Physical Properties

Property code	Value	Unit	Source
chs	-3119.60 ± 4.20	kJ/mol	NIST Webbook
gf	218.66	kJ/mol	Joback Method
hf	211.63	kJ/mol	Joback Method
hfus	13.76	kJ/mol	Joback Method
hvap	50.63	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	2.896		Crippen Method
mcvol	123.280	ml/mol	McGowan Method
pc	4316.89	kPa	Joback Method
rinpol	1431.00		NIST Webbook
ripol	2161.00		NIST Webbook
tb	558.20	K	NIST Webbook
tc	852.28	K	Joback Method
tf	310.00 ± 1.50	K	NIST Webbook
tf	307.35 ± 0.50	K	NIST Webbook
tf	308.00 ± 1.50	K	NIST Webbook
vc	0.440	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.79	J/mol×K	852.28	Joback Method

cpg	177.80	J/molxK	554.62	Joback Method
cpg	185.61	J/molxK	604.23	Joback Method
cpg	192.55	J/molxK	653.84	Joback Method
cpg	198.74	J/molxK	703.45	Joback Method
cpg	204.27	J/molxK	753.06	Joback Method
cpg	209.25	J/molxK	802.67	Joback Method
dvisc	0.0003330	Paxs	554.62	Joback Method
dvisc	0.0029814	Paxs	312.44	Joback Method
dvisc	0.0016788	Paxs	352.80	Joback Method
dvisc	0.0010637	Paxs	393.17	Joback Method
dvisc	0.0007337	Paxs	433.53	Joback Method
dvisc	0.0005391	Paxs	473.89	Joback Method
dvisc	0.0004158	Paxs	514.26	Joback Method
hfust	15.94	kJ/mol	307.35	NIST Webbook
hfust	15.93	kJ/mol	307.40	NIST Webbook
hfust	15.93	kJ/mol	307.40	NIST Webbook
sfust	51.90	J/molxK	307.35	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51398e+01
Coeff. B	-4.85971e+03
Coeff. C	-9.63160e+01
Temperature range (K), min.	423.52
Temperature range (K), max.	590.77

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C626006&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

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
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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