

1,3-DICHLORO-4-IODOBENZENE

Other names:	1,3-Dichloro-4-iodobenzene Benzene, 2,4-dichloro-1-iodo- 2,4-Dichloro-1-iodobenzene
Inchi:	InChI=1S/C6H3Cl2I/c7-4-1-2-6(9)5(8)3-4/h1-3H
InchiKey:	ZQKJCBDCOGLKCQ-UHFFFAOYSA-N
Formula:	C6H3Cl2I
SMILES:	Clc1ccc(I)c(Cl)c1
Mol. weight [g/mol]:	272.90

Physical Properties

Property code	Value	Unit	Source
hf	122.72	kJ/mol	Cheméo Relay (1.0)
hfus	17.36	kJ/mol	Joback Method
hvap	62.45	kJ/mol	Cheméo Relay (1.0)
ie	8.62	eV	Cheméo Relay (1.0)
log10ws	-4.58		Cheméo Relay (1.0)
logp	3.598		Crippen Method
mcvol	121.940	ml/mol	McGowan Method
tb	535.70	K	NIST Webbook
tf	309.24	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.10	J/mol×K	541.32	Joback Method
cpg	189.09	J/mol×K	586.39	Joback Method
cpg	195.43	J/mol×K	631.45	Joback Method
cpg	201.20	J/mol×K	676.52	Joback Method
cpg	206.42	J/mol×K	721.58	Joback Method
cpg	211.17	J/mol×K	766.65	Joback Method
cpg	215.48	J/mol×K	811.72	Joback Method
dvisc	0.0020077	Pa×s	326.74	Joback Method
dvisc	0.0012748	Pa×s	362.50	Joback Method
dvisc	0.0008782	Pa×s	398.27	Joback Method

dvisc	0.0006433	Pa×s	434.03	Joback Method
dvisc	0.0004941	Pa×s	469.79	Joback Method
dvisc	0.0003940	Pa×s	505.56	Joback Method
dvisc	0.0003237	Pa×s	541.32	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C29898326&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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