1,4-DICHLORO-2-IODOBENZENE

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

Physical Properties

Property code	Value	Unit	Source
hf	124.73	kJ/mol	Cheméo Relay (1.0)
hfus	17.36	kJ/mol	Joback Method
hvap	62.81	kJ/mol	Cheméo Relay (1.0)
ie	8.70	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	535.52	K	Cheméo Relay (1.0)
tf	299.85	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	528.70	K	98.90	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29682415&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

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
tbrp: Boiling point at reduced pressure
tf: Normal melting (fusion) point

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