

1,4-Dichloro-2-iodobenzene

Other names:	2,5-Dichloriodobenzene 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
CAS:	29682-41-5

Physical Properties

Property code	Value	Unit	Source
gf	127.05	kJ/mol	Joback Method
hf	91.81	kJ/mol	Joback Method
hfus	17.36	kJ/mol	Joback Method
hvap	50.69	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	3.598		Crippen Method
mcvol	121.940	ml/mol	McGowan Method
pc	3960.52	kPa	Joback Method
tb	541.32	K	Joback Method
tc	811.72	K	Joback Method
tf	326.74	K	Joback Method
vc	0.450	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.10	J/mol×K	541.32	Joback Method
cpg	211.17	J/mol×K	766.65	Joback Method
cpg	206.42	J/mol×K	721.58	Joback Method
cpg	201.20	J/mol×K	676.52	Joback Method
cpg	195.43	J/mol×K	631.45	Joback Method
cpg	189.09	J/mol×K	586.39	Joback Method
cpg	215.48	J/mol×K	811.72	Joback Method

dvisc	0.0003237	Paxs	541.32	Joback Method
dvisc	0.0003940	Paxs	505.56	Joback Method
dvisc	0.0004941	Paxs	469.79	Joback Method
dvisc	0.0006433	Paxs	434.03	Joback Method
dvisc	0.0008782	Paxs	398.27	Joback Method
dvisc	0.0012748	Paxs	362.50	Joback Method
dvisc	0.0020077	Paxs	326.74	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	528.70	K	98.90	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=C29682415&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mccvol:	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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