2,6-Dichloroiodobenzene

Inchi: InChI=1S/C6H3Cl2I/c7-4-2-1-3-5(8)6(4)9/h1-3H
InchiKey: ZMPGXSFTXBOKFM-UHFFFAOYSA-N
Formula: C6H3Cl2I
SMILES: Clc1cccc(Cl)c1I
Mol. weight [g/mol]: 272.90
CAS: 19230-28-5

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	m3/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	Pa×s	541.32	Joback Method
dvisc	0.0003940	Pa×s	505.56	Joback Method

dvisc	0.0004941	Pa×s	469.79	Joback Method
dvisc	0.0006433	Pa×s	434.03	Joback Method
dvisc	0.0008782	Pa×s	398.27	Joback Method
dvisc	0.0012748	Pa×s	362.50	Joback Method
dvisc	0.0020077	Pa×s	326.74	Joback Method

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=C19230285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume