2,6-Diiodophenol

Inchi: InChI=1S/C6H4I2O/c7-4-2-1-3-5(8)6(4)9/h1-3,9H
InchiKey: VMGBDTCTVUUNAO-UHFFFAOYSA-N
Formula: C6H4I2O
SMILES: Oc1c(I)cccc1I
Mol. weight [g/mol]: 345.90

Physical Properties

Property code	Value	Unit	Source
gf	64.04	kJ/mol	Joback Method
hf	34.32	kJ/mol	Joback Method
hfus	19.54	kJ/mol	Joback Method
hvap	63.65	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.601		Crippen Method
mcvol	129.150	ml/mol	McGowan Method
pc	5304.68	kPa	Joback Method
rinpol	1546.00		NIST Webbook
tb	635.24	K	Joback Method
tc	941.97	K	Joback Method
tf	424.16	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.00	J/mol×K	635.24	Joback Method
cpg	216.15	J/mol×K	686.36	Joback Method
cpg	221.65	J/mol×K	737.48	Joback Method
cpg	226.74	J/mol×K	788.60	Joback Method
cpg	231.62	J/mol×K	839.73	Joback Method
cpg	236.53	J/mol×K	890.85	Joback Method
cpg	241.67	J/mol×K	941.97	Joback Method
dvisc	0.0010426	Pa×s	424.16	Joback Method
dvisc	0.0004990	Pa×s	459.34	Joback Method

dvisc	0.0002652	Pa×s	494.52	Joback Method
dvisc	0.0001533	Pa×s	529.70	Joback Method
dvisc	0.0000949	Pa×s	564.88	Joback Method
dvisc	0.0000621	Pa×s	600.06	Joback Method
dvisc	0.0000426	Pa×s	635.24	Joback Method

Sources

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=R631902&Units=SI
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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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