1,2-Diiodopropane

Inchi: InChI=1S/C3H6I2/c1-3(5)2-4/h3H,2H2,1H3
InchiKey: ISXPOEJSKALLKA-GSVOUGTGSA-N
Formula: C3H6I2
SMILES: CC(I)CI
Mol. weight [g/mol]: 295.89
CAS: 598-29-8

Physical Properties

Property code	Value	Unit	Source
af	0.2370		KDB
gf	88.18	kJ/mol	Joback Method
hf	35.60 ± 3.40	kJ/mol	NIST Webbook
hfus	8.81	kJ/mol	Joback Method
hvap	40.63	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.245		Crippen Method
mcvol	104.770	ml/mol	McGowan Method
pc	4210.00	kPa	KDB
tb	500.20	K	KDB
tc	780.50	K	KDB
tf	253.00	K	KDB
vc	0.373	m3/kmol	KDB
zc	0.2423050		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	137.82	J/mol×K	453.88	Joback Method
cpg	144.30	J/mol×K	496.28	Joback Method
cpg	150.24	J/mol×K	538.68	Joback Method
cpg	155.69	J/mol×K	581.08	Joback Method
cpg	160.68	J/mol×K	623.48	Joback Method
cpg	165.28	J/mol×K	665.87	Joback Method
cpg	169.53	J/mol×K	708.27	Joback Method

dvisc	0.0089133	Pa×s	224.69	Joback Method
dvisc	0.0037433	Pa×s	262.89	Joback Method
dvisc	0.0019592	Pa×s	301.09	Joback Method
dvisc	0.0011863	Pa×s	339.28	Joback Method
dvisc	0.0007951	Pa×s	377.48	Joback Method
dvisc	0.0005736	Pa×s	415.68	Joback Method
dvisc	0.0004372	Pa×s	453.88	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1591
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598298&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af:	Acentric Factor
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
zc:	Critical Compressibility