

1,3-Diiodocyclobutane

Inchi:	InChI=1S/C4H6I2/c5-3-1-4(6)2-3/h3-4H,1-2H2
InchiKey:	YHRNIJSEINOLJF-UHFFFAOYSA-N
Formula:	C4H6I2
SMILES:	IC1CC(I)C1
Mol. weight [g/mol]:	307.90
CAS:	89066-32-0

Physical Properties

Property code	Value	Unit	Source
gf	139.98	kJ/mol	Joback Method
hf	193.00 ± 8.40	kJ/mol	NIST Webbook
hfl	135.00 ± 6.30	kJ/mol	NIST Webbook
hfus	12.03	kJ/mol	Joback Method
hvap	58.60 ± 4.20	kJ/mol	NIST Webbook
log10ws	-3.51		Crippen Method
logp	2.387		Crippen Method
mcvol	108.000	ml/mol	McGowan Method
pc	4305.56	kPa	Joback Method
tb	483.54	K	Joback Method
tc	759.56	K	Joback Method
tf	261.14	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	158.75	J/molxK	483.54	Joback Method
cpg	168.72	J/molxK	529.54	Joback Method
cpg	177.73	J/molxK	575.55	Joback Method
cpg	185.89	J/molxK	621.55	Joback Method
cpg	193.27	J/molxK	667.55	Joback Method
cpg	199.98	J/molxK	713.56	Joback Method
cpg	206.10	J/molxK	759.56	Joback Method
dvisc	0.0031265	Paxs	261.14	Joback Method

dvisc	0.0020884	Paxs	298.21	Joback Method
dvisc	0.0015252	Paxs	335.27	Joback Method
dvisc	0.0011857	Paxs	372.34	Joback Method
dvisc	0.0009649	Paxs	409.41	Joback Method
dvisc	0.0008125	Paxs	446.47	Joback Method
dvisc	0.0007024	Paxs	483.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C89066320&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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

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