Naphthalene, 2-iodo-

Other names: «beta»-Iodonaphthalene
Inchi: InChI=1S/C10H7I/c11-10-6-5-8-3-1-2-4-9(8)7-10/h1-7H
InchiKey: FRNLBIWVMVNNAZ-UHFFFAOYSA-N
Formula: C10H7I
SMILES: Ic1ccc2ccccc2c1
Mol. weight [g/mol]: 254.07
CAS: 612-55-5

Physical Properties

Property code	Value	Unit	Source
chs	-5079.80 ± 6.30	kJ/mol	NIST Webbook
gf	300.87	kJ/mol	Joback Method
hf	235.00 ± 9.20	kJ/mol	NIST Webbook
hfs	144.00 ± 6.30	kJ/mol	NIST Webbook
hfus	16.73	kJ/mol	Joback Method
hsub	90.80 ± 6.70	kJ/mol	NIST Webbook
hvap	51.80	kJ/mol	Joback Method
log10ws	-4.42		Crippen Method
logp	3.444		Crippen Method
mcvol	134.360	ml/mol	McGowan Method
pc	3722.56	kPa	Joback Method
tb	571.98	K	Joback Method
tc	846.27	K	Joback Method
tf	327.50 ± 0.50	K	NIST Webbook
vc	0.497	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.13	J/mol×K	571.98	Joback Method
cpg	265.95	J/mol×K	617.70	Joback Method
cpg	276.61	J/mol×K	663.41	Joback Method
cpg	286.25	J/mol×K	709.13	Joback Method
cpg	294.99	J/mol×K	754.84	Joback Method

cpg	302.96	J/mol×K	800.56	Joback Method
cpg	310.30	J/mol×K	846.27	Joback Method
dvisc	0.0013681	Pa×s	372.13	Joback Method
dvisc	0.0020777	Pa×s	332.16	Joback Method
dvisc	0.0009769	Pa×s	412.10	Joback Method
dvisc	0.0007404	Pa×s	452.07	Joback Method
dvisc	0.0005870	Pa×s	492.04	Joback Method
dvisc	0.0004819	Pa×s	532.01	Joback Method
dvisc	0.0004067	Pa×s	571.98	Joback Method
hfust	16.04	kJ/mol	327.60	NIST Webbook
hfust	16.04	kJ/mol	327.60	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	445.20	K	2.80	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C612555&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature

hsub:	Enthalpy of sublimation 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume