Benzene, 2-iodo-1,3-dimethyl-

Other names:	1,3-dimethyl-2-iodobenzene
	1-iodo-2,6-dimethylbenzene
	2,6-Dimethyliodobenzene
	2-iodo-1,3-dimethylbenzene
	2-iodo-m-xylene
	benzene, 1-iodo-2,6-dimethyl-
	m-xylene, 2-iodo-
Inchi:	InChI=1S/C8H9I/c1-6-4-3-5-7(2)8(6)9/h3-5H,1-2H3
InchiKey:	QTUGGVBKWIYQSS-UHFFFAOYSA-N
Formula:	C8H9I
SMILES:	Cc1cccc(C)c1I
Mol. weight [g/mol]:	232.06
CAS:	608-28-6

Physical Properties

Property code	Value	Unit	Source
gf	167.75	kJ/mol	Joback Method
hf	82.01	kJ/mol	Joback Method
hfus	14.14	kJ/mol	Joback Method
hvap	46.38	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	2.908		Crippen Method
mcvol	125.640	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	502.70	K	NIST Webbook
tc	761.77	K	Joback Method
tf	284.33 ± 0.30	K	NIST Webbook
vc	0.464	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	222.94	J/mol×K	512.22	Joback Method
cpg	234.35	J/mol×K	553.81	Joback Method

cpg	244.98	J/mol×K	595.40	Joback Method
cpg	254.87	J/mol×K	637.00	Joback Method
cpg	264.08	J/mol×K	678.59	Joback Method
cpg	272.63	J/mol×K	720.18	Joback Method
cpg	280.59	J/mol×K	761.77	Joback Method
dvisc	0.0021926	Pa×s	289.44	Joback Method
dvisc	0.0012902	Pa×s	326.57	Joback Method
dvisc	0.0008460	Pa×s	363.70	Joback Method
dvisc	0.0005998	Pa×s	400.83	Joback Method
dvisc	0.0004508	Pa×s	437.96	Joback Method
dvisc	0.0003543	Pa×s	475.09	Joback Method
dvisc	0.0002884	Pa×s	512.22	Joback Method
pvap	0.01	kPa	296.50	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	7.09e-03	kPa	288.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	9.25e-03	kPa	291.60	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	5.00e-03	kPa	284.50	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.02	kPa	298.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.02	kPa	299.50	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.02	kPa	301.50	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.02	kPa	303.30	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.03	kPa	306.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.03	kPa	308.30	Thermochemistry of Halogen-Substituted Methylbenzenes

pvap	0.04	kPa	311.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.05	kPa	313.60	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.06	kPa	316.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.07	kPa	318.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.08	kPa	321.20	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.09	kPa	323.40	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.11	kPa	326.30	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.13	kPa	328.50	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.15	kPa	331.30	Thermochemistry of Halogen-Substituted Methylbenzenes
pvap	0.17	kPa	333.40	Thermochemistry of Halogen-Substituted Methylbenzenes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	375.70	K	1.90	NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermochemistry of Halogen-Substituted Methylbenzenes:	https://www.doi.org/10.1021/je500784s
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=C608286&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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume