

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: Cc1ccccc(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	Paxs	289.44	Joback Method
dvisc	0.0012902	Paxs	326.57	Joback Method
dvisc	0.0008460	Paxs	363.70	Joback Method
dvisc	0.0005998	Paxs	400.83	Joback Method
dvisc	0.0004508	Paxs	437.96	Joback Method
dvisc	0.0003543	Paxs	475.09	Joback Method
dvisc	0.0002884	Paxs	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

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
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
mvol:	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

Latest version available from:

<https://www.chemeo.com/cid/54-059-7/Benzene-2-iodo-1-3-dimethyl.pdf>

Generated by Cheméo on 2024-04-10 07:25:50.80676873 +0000 UTC m=+15023199.727346043.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.