

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

Other names:	1,2-dimethyl-3-iodobenzene
Inchi:	InChI=1S/C8H9I/c1-6-4-3-5-8(9)7(6)2/h3-5H,1-2H3
InchiKey:	DANMWBNOPFBJSZ-UHFFFAOYSA-N
Formula:	C8H9I
SMILES:	Cc1cccc(I)c1C
Mol. weight [g/mol]:	232.06
CAS:	31599-60-7

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	502.20	K	NIST Webbook
tc	761.77	K	Joback Method
tf	289.44	K	Joback Method
vc	0.464	m ³ /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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	398.70	K	2.00	NIST Webbook

Sources

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=C31599607&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307i
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
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

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