

# Benzene, 1-iodo-4-(trifluoromethyl)-

<b>Other names:</b>	p-Iodobenzotrifluoride «alpha», «alpha», «alpha»-trifluoro-4-iodotoluene
<b>Inchi:</b>	InChI=1S/C7H4F3I/c8-7(9,10)5-1-3-6(11)4-2-5/h1-4H
<b>InchiKey:</b>	SKGRFPGOGCHDPC-UHFFFAOYSA-N
<b>Formula:</b>	C7H4F3I
<b>SMILES:</b>	FC(F)(F)c1ccc(I)cc1
<b>Mol. weight [g/mol]:</b>	272.01
<b>CAS:</b>	455-13-0

## Physical Properties

Property code	Value	Unit	Source
gf	-412.63	kJ/mol	Joback Method
hf	-482.96	kJ/mol	Joback Method
hfus	13.77	kJ/mol	Joback Method
hvap	39.74	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.310		Crippen Method
mcvol	116.860	ml/mol	McGowan Method
pc	3411.87	kPa	Joback Method
tb	458.50 ± 0.50	K	NIST Webbook
tc	707.75	K	Joback Method
tf	269.84	K	Joback Method
vc	0.451	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.40	J/mol×K	478.94	Joback Method
cpg	221.30	J/mol×K	517.08	Joback Method
cpg	230.28	J/mol×K	555.21	Joback Method
cpg	238.43	J/mol×K	593.35	Joback Method
cpg	245.80	J/mol×K	631.48	Joback Method
cpg	252.48	J/mol×K	669.62	Joback Method
cpg	258.51	J/mol×K	707.75	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.70	K	99.30	NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C455130&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C455130&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvp:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/11-762-3/Benzene-1-iodo-4-trifluoromethyl.pdf>

Generated by Cheméo on 2024-04-24 13:27:45.74921445 +0000 UTC m=+16254514.669791765.

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