Benzene, 1-iodo-3-(trifluoromethyl)-

Other names:	m-Iodobenzotrifluoride
	3-Iodobenzotrifluoride
	3-(Trifluoromethyl)iodobenzene
	«alpha»,«alpha»,«alpha»-Trifluoro-m-iodotoluene
	m-(Trifluoromethyl)iodobenzene
	Toluene, «alpha»,«alpha»,«alpha»-trifluoro-m-iodo-
	1-Iodo-3-(trifluoromethyl)benzene
	m-Iodo-«alpha»,«alpha»,«alpha»-trifluorotoluene
Inchi:	InChI=1S/C7H4F3I/c8-7(9,10)5-2-1-3-6(11)4-5/h1-4H
InchiKey:	IGISPMBUGPHLBY-UHFFFAOYSA-N
Formula:	C7H4F3I
SMILES:	FC(F)(F)c1cccc(I)c1
Mol. weight [g/mol]:	272.01
CAS:	401-81-0

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
rinpol	1015.60		NIST Webbook
rinpol	1023.00		NIST Webbook
rinpol	1015.60		NIST Webbook
tb	478.94	K	Joback Method
tc	707.75	K	Joback Method
tf	269.84	K	Joback Method
vc	0.451	m3/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	355.50	K	3.30	NIST Webbook
tbrp	355.00	K	3.30	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=C401810&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg: Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume