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

Other names:	p-Iodobenzotrifluoride
	«alpha»,«alpha»,«alpha»-trifluoro-4-iodotoluene
Inchi:	InChI=1S/C7H4F3I/c8-7(9,10)5-1-3-6(11)4-2-5/h1-4H
InchiKey:	SKGRFPGOGCHDPC-UHFFFAOYSA-N
Formula:	C7H4F3I
SMILES:	FC(F)(F)c1ccc(I)cc1
Mol. weight [g/mol]:	272.01
CAS:	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	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	458.70	K	99.30	NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C455130&Units=SI

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
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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