4-Chloro-3-iodobenzotrifluoride

Other names: Benzene, 1-chloro-2-iodo-4-(trifluoromethyl)-
Toluene, 4-chloro-3-iodo-alpha,alpha,alpha-trifluoro-
4-Chloro-3-iodo-«alpha»,«alpha»,«alpha»-trifluorotoluene
1-chloro-2-iodo-4-(trifluoromethyl)benzene
Inchi: InChI=1S/C7H3ClF3I/c8-5-2-1-4(3-6(5)12)7(9,10)11/h1-3H
InchiKey: SSLWFPKNYZEOTH-UHFFFAOYSA-N
Formula: C7H3ClF3I
SMILES: FC(F)(F)c1ccc(Cl)c(I)c1
Mol. weight [g/mol]: 306.45
CAS: 672-57-1

Physical Properties

Property code	Value	Unit	Source
gf	-434.19	kJ/mol	Joback Method
hf	-510.17	kJ/mol	Joback Method
hfus	17.58	kJ/mol	Joback Method
hvap	44.79	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.963		Crippen Method
mcvol	129.100	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
rinpol	1170.80		NIST Webbook
rinpol	1170.80		NIST Webbook
tb	521.35	K	Joback Method
tc	756.83	K	Joback Method
tf	312.28	K	Joback Method
vc	0.499	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.49	J/mol×K	521.35	Joback Method
cpg	240.98	J/mol×K	560.60	Joback Method
cpg	248.67	J/mol×K	599.84	Joback Method

cpg	255.60	J/mol×K	639.09	Joback Method
cpg	261.85	J/mol×K	678.34	Joback Method
cpg	267.48	J/mol×K	717.59	Joback Method
cpg	272.57	J/mol×K	756.83	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	332.20	K	0.07	NIST Webbook
tbrp	332.00 ± 1.00	K	0.07	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=C672571&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
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