Benzoic acid, 2,3,5-triiodo-

Other names:	Floraltone
	Johnkolor
	Triiodobenzoic acid
	TIB
	TIBA
	2,3,5-Triiodobenzoic acid
	2,3,5-TIBA
	Regin 8
	Kyselina 2,3,5-trijodbenzoova
	A 20812
	NSC 2582
Inchi:	InChI=1S/C7H3I3O2/c8-3-1-4(7(11)12)6(10)5(9)2-3/h1-2H,(H,11,12)
InchiKey:	ZMZGFLUUZLELNE-UHFFFAOYSA-N
Formula:	C7H3I3O2
SMILES:	O=C(O)c1cc(I)cc(I)c1I
Mol. weight [g/mol]:	499.81
CAS:	88-82-4

Physical Properties

Property code	Value	Unit	Source
gf	0.20	kJ/mol	Joback Method
hf	-19.89	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	86.98	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	3.199		Crippen Method
mcvol	170.630	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
tb	826.65	K	Joback Method
tc	1116.48	K	Joback Method
tf	503.80 ± 0.20	K	NIST Webbook
vc	0.609	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	273.27	J/mol×K	826.65	Joback Method
cpg	277.72	J/mol×K	874.95	Joback Method
cpg	281.85	J/mol×K	923.26	Joback Method
cpg	285.77	J/mol×K	971.56	Joback Method
cpg	289.58	J/mol×K	1019.87	Joback Method
cpg	293.36	J/mol×K	1068.17	Joback Method
cpg	297.22	J/mol×K	1116.48	Joback Method
dvisc	0.0003346	Pa×s	569.07	Joback Method
dvisc	0.0006597	Pa×s	517.56	Joback Method
dvisc	0.0001900	Pa×s	620.59	Joback Method
dvisc	0.0001176	Pa×s	672.11	Joback Method
dvisc	0.0000780	Pa×s	723.62	Joback Method
dvisc	0.0000546	Pa×s	775.13	Joback Method
dvisc	0.0000400	Pa×s	826.65	Joback Method
hfust	32.23	kJ/mol	503.80	NIST Webbook
hfust	32.23	kJ/mol	503.80	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=C88824&Units=SI

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
hfust: Enthalpy of fusion at a given temperature

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume