Benzenamine, 2,4,6-tribromo-

Other names:	Aniline, 2,4,6-tribromo- s-Tribromoaniline 2,4,6-Tribromoaniline 2,4,6-Tribomoaniline 2,4,6-Tribromoanine USAF do-43 2,4,6-Tribromophenylamine sym-Tribromoaniline 2,4,6-Tribromobenzenamine
Inchi:	InChI=1S/C6H4Br3N/c7-3-1-4(8)6(10)5(9)2-3/h1-2H,10H2
InchiKey:	GVPODVKBTHCGFU-UHFFFAOYSA-N
Formula:	C6H4Br3N
SMILES:	Nc1c(Br)cc(Br)cc1Br
Mol. weight [g/mol]:	329.81
CAS:	147-82-0

Physical Properties

Property code	Value	Unit	Source
chs	-2988.60 ± 3.20	kJ/mol	NIST Webbook
gf	192.57	kJ/mol	Joback Method
hf	159.00 ± 2.60	kJ/mol	NIST Webbook
hfs	57.90 ± 2.40	kJ/mol	NIST Webbook
hfus	25.22	kJ/mol	Joback Method
hsub	101.10 ± 1.10	kJ/mol	NIST Webbook
hsub	96.70 ± 1.70	kJ/mol	NIST Webbook
hvap	63.16	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.556		Crippen Method
mcvol	134.120	ml/mol	McGowan Method
pc	6461.89	kPa	Joback Method
rinpol	1646.00		NIST Webbook
rinpol	1642.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1644.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1648.00		NIST Webbook

rinpol	1635.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1646.00		NIST Webbook
tb	573.20	K	NIST Webbook
tc	930.26	K	Joback Method
tf	395.00 ± 3.00	K	NIST Webbook
tf	393.00 ± 3.00	K	NIST Webbook
tf	394.85 ± 0.25	K	NIST Webbook
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	254.04	J/mol×K	883.43	Joback Method
cpg	227.02	J/mol×K	649.31	Joback Method
cpg	233.42	J/mol×K	696.13	Joback Method
cpg	239.24	J/mol×K	742.96	Joback Method
cpg	244.57	J/mol×K	789.78	Joback Method
cpg	249.48	J/mol×K	836.61	Joback Method
cpg	258.34	J/mol×K	930.26	Joback Method
cps	181.40	J/mol×K	298.15	NIST Webbook
hfust	25.75	kJ/mol	393.00	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=C147820&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
cps: Solid phase heat capacity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume