Tribromochloromethane

Inchi: InChI=1S/CBr3Cl/c2-1(3,4)5
InchiKey: GKXZMEXQUWZGJK-UHFFFAOYSA-N
Formula: CBr3Cl
SMILES: ClC(Br)(Br)Br
Mol. weight [g/mol]: 287.18
CAS: 594-15-0

Physical Properties

Property code	Value	Unit	Source
gf	-8.59	kJ/mol	Joback Method
hf	-9.47	kJ/mol	Joback Method
hfus	10.98	kJ/mol	Joback Method
hvap	40.21	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.021		Crippen Method
mcvol	89.690	ml/mol	McGowan Method
pc	7901.23	kPa	Joback Method
rinpol	955.00		NIST Webbook
tb	377.45 ± 0.60	K	NIST Webbook
tc	715.52	K	Joback Method
tf	312.77	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	99.25	J/mol×K	454.96	Joback Method
cpg	101.63	J/mol×K	498.39	Joback Method
cpg	103.40	J/mol×K	541.81	Joback Method
cpg	104.65	J/mol×K	585.24	Joback Method
cpg	105.47	J/mol×K	628.67	Joback Method
cpg	105.95	J/mol×K	672.10	Joback Method
cpg	106.18	J/mol×K	715.52	Joback Method
dvisc	0.0029648	Pa×s	312.77	Joback Method

dvisc	0.0020351	Pa×s	336.47	Joback Method
dvisc	0.0014679	Pa×s	360.17	Joback Method
dvisc	0.0011023	Pa×s	383.87	Joback Method
dvisc	0.0008558	Pa×s	407.56	Joback Method
dvisc	0.0006832	Pa×s	431.26	Joback Method
dvisc	0.0005584	Pa×s	454.96	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61421e+01
Coeff. B	-4.34965e+03
Temperature range (K), min.	274.35
Temperature range (K), max.	401.64

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C594150&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume