

Propane, 1,2,3-tribromo-

Other names:	1,2,3-Tribromopropane Glycerol tribromohydrin Glyceryl tribromohydrin s-Tribromopropane sym-Tribromopropane
Inchi:	InChI=1S/C3H5Br3/c4-1-3(6)2-5/h3H,1-2H2
InchiKey:	FHCLGDLYRUPKAM-UHFFFAOYSA-N
Formula:	C3H5Br3
SMILES:	BrCC(Br)CBr
Mol. weight [g/mol]:	280.78
CAS:	96-11-7

Physical Properties

Property code	Value	Unit	Source
gf	14.90	kJ/mol	Joback Method
hf	-31.54	kJ/mol	Joback Method
hfus	15.86	kJ/mol	Joback Method
hvap	41.19	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	2.540		Crippen Method
mcvol	105.630	ml/mol	McGowan Method
pc	5999.95	kPa	Joback Method
rinpol	1148.00		NIST Webbook
tb	495.30	K	NIST Webbook
tb	493.20	K	NIST Webbook
tc	699.87	K	Joback Method
tf	289.30 ± 0.02	K	NIST Webbook
tf	285.41 ± 0.05	K	NIST Webbook
vc	0.384	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	174.17	J/mol×K	660.91	Joback Method

cpg	165.43	J/molxK	582.98	Joback Method
cpg	160.46	J/molxK	544.01	Joback Method
cpg	155.03	J/molxK	505.05	Joback Method
cpg	149.10	J/molxK	466.08	Joback Method
cpg	169.98	J/molxK	621.94	Joback Method
cpg	178.04	J/molxK	699.87	Joback Method
cpl	166.50	J/molxK	298.00	NIST Webbook
dvisc	0.0032395	Paxs	287.97	Joback Method
dvisc	0.0004514	Paxs	466.08	Joback Method
dvisc	0.0005607	Paxs	436.39	Joback Method
dvisc	0.0007188	Paxs	406.71	Joback Method
dvisc	0.0009582	Paxs	377.02	Joback Method
dvisc	0.0013417	Paxs	347.34	Joback Method
dvisc	0.0020007	Paxs	317.66	Joback Method
hfust	23.78	kJ/mol	289.40	NIST Webbook
hfust	23.78	kJ/mol	289.40	NIST Webbook
hvapt	50.20	kJ/mol	439.00	NIST Webbook
hvapt	50.80	kJ/mol	492.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53100e+01
Coeff. B	-4.43013e+03
Coeff. C	-7.88460e+01
Temperature range (K), min.	373.75
Temperature range (K), max.	524.73

Sources

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=C96117&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/ci9903071

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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