

Propane, 1,1,2-tribromo-

Other names:	1,1,2-Tribromopropane
Inchi:	InChI=1S/C3H5Br3/c1-2(4)3(5)6/h2-3H,1H3
InchiKey:	ZLOLQHBVMYXNHX-UHFFFAOYSA-N
Formula:	C3H5Br3
SMILES:	CC(Br)C(Br)Br
Mol. weight [g/mol]:	280.78
CAS:	14602-62-1

Physical Properties

Property code	Value	Unit	Source
gf	12.46	kJ/mol	Joback Method
hf	-36.82	kJ/mol	Joback Method
hfus	12.33	kJ/mol	Joback Method
hvap	40.80	kJ/mol	Joback Method
log10ws	-3.09		Crippen Method
logp	2.886		Crippen Method
mcvol	105.630	ml/mol	McGowan Method
pc	6075.01	kPa	Joback Method
tb	465.64	K	Joback Method
tc	705.27	K	Joback Method
tf	272.97	K	Joback Method
vc	0.378	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.36	J/mol×K	465.64	Joback Method
cpg	155.53	J/mol×K	505.58	Joback Method
cpg	161.17	J/mol×K	545.52	Joback Method
cpg	166.31	J/mol×K	585.46	Joback Method
cpg	171.01	J/mol×K	625.39	Joback Method
cpg	175.32	J/mol×K	665.33	Joback Method
cpg	179.28	J/mol×K	705.27	Joback Method
dvisc	0.0043204	Paxs	272.97	Joback Method

dvisc	0.0024016	Paxs	305.08	Joback Method
dvisc	0.0014929	Paxs	337.19	Joback Method
dvisc	0.0010081	Paxs	369.31	Joback Method
dvisc	0.0007248	Paxs	401.42	Joback Method
dvisc	0.0005472	Paxs	433.53	Joback Method
dvisc	0.0004295	Paxs	465.64	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49957e+01
Coeff. B	-4.17498e+03
Coeff. C	-7.29640e+01
Temperature range (K), min.	356.82
Temperature range (K), max.	504.08

Sources

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/ci990307i
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=C14602621&Units=SI

Legend

cp_g:	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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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