

Propane, 2-methyl-1,2,3-tribromo-

Other names:	1,2,3-tribromo-2-methylpropane
Inchi:	InChI=1S/C4H7Br3/c1-4(7,2-5)3-6/h2-3H2,1H3
InchiKey:	OIRQLILPXCJMIY-UHFFFAOYSA-N
Formula:	C4H7Br3
SMILES:	CC(Br)(CBr)CBr
Mol. weight [g/mol]:	294.81
CAS:	631-28-7

Physical Properties

Property code	Value	Unit	Source
gf	28.60	kJ/mol	Joback Method
hf	-55.65	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	42.51	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.930		Crippen Method
mcvol	119.720	ml/mol	McGowan Method
pc	5281.57	kPa	Joback Method
tb	486.17	K	Joback Method
tc	726.33	K	Joback Method
tf	316.66	K	Joback Method
vc	0.434	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	189.99	J/molxK	486.17	Joback Method
cpg	197.96	J/molxK	526.20	Joback Method
cpg	205.14	J/molxK	566.22	Joback Method
cpg	211.61	J/molxK	606.25	Joback Method
cpg	217.45	J/molxK	646.28	Joback Method
cpg	222.74	J/molxK	686.30	Joback Method
cpg	227.56	J/molxK	726.33	Joback Method
dvisc	0.0029905	Paxs	316.66	Joback Method

dvisc	0.0018861	Paxs	344.91	Joback Method
dvisc	0.0012755	Paxs	373.16	Joback Method
dvisc	0.0009115	Paxs	401.41	Joback Method
dvisc	0.0006807	Paxs	429.67	Joback Method
dvisc	0.0005270	Paxs	457.92	Joback Method
dvisc	0.0004204	Paxs	486.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.52873e+01
Coeff. B	-4.40652e+03
Coeff. C	-7.82460e+01
Temperature range (K), min.	372.02
Temperature range (K), max.	522.47

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C631287&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
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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