Propane, 2,2-dibromo-

Other names: 2,2-Dibromopropane
Inchi: InChI=1S/C3H6Br2/c1-3(2,4)5/h1-2H3
InchiKey: ARITXYXYCOZKMU-UHFFFAOYSA-N
Formula: C3H6Br2
SMILES: CC(C)(Br)Br
Mol. weight [g/mol]: 201.89
CAS: 594-16-1

Physical Properties

Property code	Value	Unit	Source
gf	5.86	kJ/mol	Joback Method
hf	-61.34	kJ/mol	Joback Method
hfus	6.68	kJ/mol	Joback Method
hvap	33.85	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.512		Crippen Method
mcvol	88.130	ml/mol	McGowan Method
pc	5495.11	kPa	Joback Method
rinpol	771.00		NIST Webbook
rinpol	771.00		NIST Webbook
tb	397.13	K	Joback Method
tc	620.94	K	Joback Method
tf	245.59	K	Joback Method
vc	0.317	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	125.78	J/mol×K	397.13	Joback Method
cpg	133.21	J/mol×K	434.43	Joback Method
cpg	139.96	J/mol×K	471.73	Joback Method
cpg	146.10	J/mol×K	509.03	Joback Method
cpg	151.67	J/mol×K	546.33	Joback Method
cpg	156.74	J/mol×K	583.64	Joback Method

cpg	161.34	J/mol×K	620.94	Joback Method
dvisc	0.0045692	Pa×s	245.59	Joback Method
dvisc	0.0026821	Pa×s	270.85	Joback Method
dvisc	0.0017242	Pa×s	296.10	Joback Method
dvisc	0.0011881	Pa×s	321.36	Joback Method
dvisc	0.0008644	Pa×s	346.62	Joback Method
dvisc	0.0006566	Pa×s	371.87	Joback Method
dvisc	0.0005165	Pa×s	397.13	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	387.70	K	98.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.39169e+01
Coeff. B	-2.70302e+03
Coeff. C	-9.75580e+01
Temperature range (K), min.	295.88
Temperature range (K), max.	411.66

Sources

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=C594161&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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume