Propane, 1,2-dibromo-2-methyl-

Other names: 1,2-Dibromo-2-methylpropane
1,2-Dibromoisobutane
Isobutylene bromide
Inchi: InChI=1S/C4H8Br2/c1-4(2,6)3-5/h3H2,1-2H3
InchiKey: SDTXSEXYPROZSZ-UHFFFAOYSA-N
Formula: C4H8Br2
SMILES: CC(C)(Br)CBr
Mol. weight [g/mol]: 215.91
CAS: 594-34-3

Physical Properties

Property code	Value	Unit	Source
gf	14.28	kJ/mol	Joback Method
hf	-113.30 ± 1.00	kJ/mol	NIST Webbook
hfl	-150.50	kJ/mol	NIST Webbook
hfl	-156.60 ± 1.00	kJ/mol	NIST Webbook
hfus	9.27	kJ/mol	Joback Method
hvap	43.37	kJ/mol	NIST Webbook
hvap	43.30 ± 0.10	kJ/mol	NIST Webbook
log10ws	-2.47		Crippen Method
logp	2.555		Crippen Method
mcvol	102.220	ml/mol	McGowan Method
pc	4789.21	kPa	Joback Method
rinpol	865.00		NIST Webbook
rinpol	893.00		NIST Webbook
rinpol	893.00		NIST Webbook
tb	423.20	K	NIST Webbook
tb	422.15 ± 0.40	K	NIST Webbook
tb	423.20	K	NIST Webbook
tc	641.12	K	Joback Method
tf	202.85 ± 0.30	K	NIST Webbook
tf	203.05 ± 0.30	K	NIST Webbook
vc	0.372	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.59	J/mol×K	604.27	Joback Method
cpg	204.42	J/mol×K	641.12	Joback Method
cpg	160.70	J/mol×K	420.01	Joback Method
cpg	169.62	J/mol×K	456.86	Joback Method
cpg	177.81	J/mol×K	493.71	Joback Method
cpg	185.34	J/mol×K	530.56	Joback Method
cpg	192.25	J/mol×K	567.41	Joback Method
dvisc	0.0004673	Pa×s	420.01	Joback Method
dvisc	0.0005981	Pa×s	392.82	Joback Method
dvisc	0.0044971	Pa×s	256.86	Joback Method
dvisc	0.0025740	Pa×s	284.05	Joback Method
dvisc	0.0016241	Pa×s	311.24	Joback Method
dvisc	0.0011035	Pa×s	338.44	Joback Method
dvisc	0.0007941	Pa×s	365.63	Joback Method
hvapt	36.52	kJ/mol	423.20	NIST Webbook
hvapt	33.30	kJ/mol	333.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.20	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38853e+01
Coeff. B	-2.95167e+03
Coeff. C	-1.04684e+02
Temperature range (K), min.	321.76
Temperature range (K), max.	448.95

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C594343&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
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
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