

1,1-Dibromopropene

Other names:	1,1-Dibromo-1-propene 1-Propene, 1,1-dibromo-
Inchi:	InChI=1S/C3H4Br2/c1-2-3(4)5/h2H,1H3
InchiKey:	HTEJLXYOJZOXKM-UHFFFAOYSA-N
Formula:	C3H4Br2
SMILES:	CC=C(Br)Br
Mol. weight [g/mol]:	199.87
CAS:	13195-80-7

Physical Properties

Property code	Value	Unit	Source
gf	74.69	kJ/mol	Joback Method
hf	54.84	kJ/mol	Joback Method
hfus	12.99	kJ/mol	Joback Method
hvap	35.18	kJ/mol	Joback Method
log10ws	-2.79		Crippen Method
logp	2.637		Crippen Method
mvol	83.830	ml/mol	McGowan Method
pc	5818.28	kPa	Joback Method
tb	404.40	K	Joback Method
tc	629.17	K	Joback Method
tf	224.13	K	Joback Method
vc	0.308	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	107.57	J/molxK	404.40	Joback Method
cpg	113.17	J/molxK	441.86	Joback Method
cpg	118.28	J/molxK	479.32	Joback Method
cpg	122.92	J/molxK	516.79	Joback Method
cpg	127.14	J/molxK	554.25	Joback Method
cpg	131.00	J/molxK	591.71	Joback Method
cpg	134.52	J/molxK	629.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.31239e+01
Coeff. B	-3.08950e+03
Coeff. C	-5.18360e+01
Temperature range (K), min.	292.52
Temperature range (K), max.	447.29

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13195807&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cp_g:	Ideal gas heat capacity
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:	Log ₁₀ 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

Latest version available from:

<https://www.cheméo.com/cid/51-437-0/1-1-Dibromopropene.pdf>

Generated by Cheméo on 2024-04-17 02:10:24.661678754 +0000 UTC m=+15609073.582256070.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.