1,1-Dibromo-1-propene

Other names: 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
hf	49.03	kJ/mol	Cheméo Relay (1.0)
hfus	12.99	kJ/mol	Joback Method
ie	8.99	eV	Cheméo Relay (1.0)
logp	2.637		Crippen Method
mcvol	83.830	ml/mol	McGowan Method
tb	395.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Correlations

Information	Value

Property code	pvap
Equation	ln(Pvp) = 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

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13195807&Units=SI
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
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature