cis-1-Bromo-1-propene

Inchi: InChI=1S/C3H5Br/c1-2-3-4/h2-3H,1H3/b3-2-
InchiKey: NNQDMQVWOWCVEM-IHWYPQMZSA-N
Formula: C3H5Br
SMILES: CC=CBr
Mol. weight [g/mol]: 120.98
CAS: 590-13-6

Physical Properties

Property code	Value	Unit	Source
gf	68.92	kJ/mol	Joback Method
hf	38.30	kJ/mol	Joback Method
hfus	9.01	kJ/mol	Joback Method
hvap	28.67	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.915		Crippen Method
mcvol	66.330	ml/mol	McGowan Method
pc	5213.15	kPa	Joback Method
rinpol	582.00		NIST Webbook
tb	338.36	K	Joback Method
tc	534.95	K	Joback Method
tf	178.29	K	Joback Method
vc	0.245	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	81.97	J/mol×K	338.36	Joback Method
cpg	87.80	J/mol×K	371.12	Joback Method
cpg	93.25	J/mol×K	403.89	Joback Method
cpg	98.35	J/mol×K	436.65	Joback Method
cpg	103.12	J/mol×K	469.42	Joback Method
cpg	107.57	J/mol×K	502.18	Joback Method
cpg	111.73	J/mol×K	534.95	Joback Method
dvisc	0.0028576	Pa×s	178.29	Joback Method

dvisc	0.0015320	Pa×s	204.97	Joback Method
dvisc	0.0009481	Pa×s	231.65	Joback Method
dvisc	0.0006479	Pa×s	258.32	Joback Method
dvisc	0.0004755	Pa×s	285.00	Joback Method
dvisc	0.0003679	Pa×s	311.68	Joback Method
dvisc	0.0002964	Pa×s	338.36	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45849e+01
Coeff. B	-2.93391e+03
Coeff. C	-3.66250e+01
Temperature range (K), min.	241.83
Temperature range (K), max.	353.00

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R596364&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume