Propane, 1-bromo-2,2-dimethyl-

Other names: (CH3)3CCH2Br
1-Bromo-2,2-dimethylpropane
Neopentyl bromide
Inchi: InChI=1S/C5H11Br/c1-5(2,3)4-6/h4H2,1-3H3
InchiKey: CQWYAXCOVZKLHY-UHFFFAOYSA-N
Formula: C5H11Br
SMILES: CC(C)(C)CBr
Mol. weight [g/mol]: 151.04
CAS: 630-17-1

Physical Properties

Property code	Value	Unit	Source
gf	8.38	kJ/mol	Joback Method
hf	-128.95	kJ/mol	Joback Method
hfus	6.58	kJ/mol	Joback Method
hvap	31.86	kJ/mol	Joback Method
ie	10.01	eV	NIST Webbook
ie	10.04 ± 0.01	eV	NIST Webbook
log10ws	-2.11		Crippen Method
logp	2.427		Crippen Method
mcvol	98.810	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
tb	379.20	K	NIST Webbook
tc	574.49	K	Joback Method
tf	208.33	K	Joback Method
vc	0.366	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.45	J/mol×K	574.49	Joback Method
cpg	162.75	J/mol×K	376.73	Joback Method
cpg	173.57	J/mol×K	409.69	Joback Method
cpg	183.72	J/mol×K	442.65	Joback Method

cpg	193.25	J/mol×K	475.61	Joback Method
cpg	202.20	J/mol×K	508.57	Joback Method
cpg	210.59	J/mol×K	541.53	Joback Method
dvisc	0.0004084	Pa×s	376.73	Joback Method
dvisc	0.0067392	Pa×s	208.33	Joback Method
dvisc	0.0032006	Pa×s	236.40	Joback Method
dvisc	0.0017803	Pa×s	264.46	Joback Method
dvisc	0.0011082	Pa×s	292.53	Joback Method
dvisc	0.0007496	Pa×s	320.60	Joback Method
dvisc	0.0005399	Pa×s	348.66	Joback Method
hvapt	35.60	kJ/mol	356.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	378.70	K	102.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.35022e+01
Coeff. B	-2.55049e+03
Coeff. C	-9.21060e+01
Temperature range (K), min.	285.11
Temperature range (K), max.	403.50

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C630171&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
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume