Butane, 2-bromo-2-methyl-

Other names:	2-Bromo-2-methylbutane
	2-Methyl-2-bromobutane
	tert-Amyl bromide
	tert-Pentyl bromide
Inchi:	InChI=1S/C5H11Br/c1-4-5(2,3)6/h4H2,1-3H3
InchiKey:	JOUWCKCVTDSMHF-UHFFFAOYSA-N
Formula:	C5H11Br
SMILES:	CCC(C)(C)Br
Mol. weight [g/mol]:	151.04
CAS:	507-36-8

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
log10ws	-2.46		Crippen Method
logp	2.570		Crippen Method
mcvol	98.810	ml/mol	McGowan Method
pc	3857.88	kPa	Joback Method
rinpol	734.00		NIST Webbook
rinpol	750.00		NIST Webbook
ripol	925.00		NIST Webbook
ripol	939.00		NIST Webbook
ripol	937.00		NIST Webbook
tb	380.00	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	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
cpg	218.45	J/mol×K	574.49	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
dvisc	0.0004084	Pa×s	376.73	Joback Method
hvapt	36.40	kJ/mol	358.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	380.20	K	98.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.36146e+01
Coeff. B	-2.58477e+03
Coeff. C	-9.26850e+01
Temperature range (K), min.	286.63
Temperature range (K), max.	403.99

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C507368&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
ripol:	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