Pentane, 3-bromo-

Other names:	3-Bromopentane
	3-Pentyl bromide
Inchi:	InChI=1S/C5H11Br/c1-3-5(6)4-2/h5H,3-4H2,1-2H3
InchiKey:	VTOQFOCYBTVOJZ-UHFFFAOYSA-N
Formula:	C5H11Br
SMILES:	CCC(Br)CC
Mol. weight [g/mol]:	151.04
CAS:	1809-10-5

Physical Properties

Property code	Value	Unit	Source
gf	3.10	kJ/mol	Joback Method
hf	-125.48	kJ/mol	Joback Method
hfus	10.47	kJ/mol	Joback Method
hvap	32.77	kJ/mol	Joback Method
log10ws	-2.46		Crippen Method
logp	2.570		Crippen Method
mcvol	98.810	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	853.00		NIST Webbook
rinpol	852.00		NIST Webbook
rinpol	851.00		NIST Webbook
ripol	994.00		NIST Webbook
ripol	997.00		NIST Webbook
ripol	1009.00		NIST Webbook
ripol	989.00		NIST Webbook
tb	391.80	K	NIST Webbook
tc	568.83	K	Joback Method
tf	190.91	K	Joback Method
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	212.94	J/mol×K	568.83	Joback Method
cpg	161.30	J/mol×K	379.52	Joback Method
cpg	170.96	J/mol×K	411.07	Joback Method
cpg	180.18	J/mol×K	442.62	Joback Method
cpg	188.97	J/mol×K	474.18	Joback Method
cpg	197.35	J/mol×K	505.73	Joback Method
cpg	205.34	J/mol×K	537.28	Joback Method
dvisc	0.0003481	Pa×s	379.52	Joback Method
dvisc	0.0061616	Pa×s	190.91	Joback Method
dvisc	0.0027207	Pa×s	222.34	Joback Method
dvisc	0.0014710	Pa×s	253.78	Joback Method
dvisc	0.0009108	Pa×s	285.21	Joback Method
dvisc	0.0006202	Pa×s	316.65	Joback Method
dvisc	0.0004527	Pa×s	348.08	Joback Method
hfust	8.40	kJ/mol	167.30	NIST Webbook
hfust	8.40	kJ/mol	167.30	NIST Webbook
hvapt	37.70	kJ/mol	369.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47451e+01
Coeff. B	-3.55117e+03
Coeff. C	-4.11270e+01
Temperature range (K), min.	286.76
Temperature range (K), max.	417.57

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1809105&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
hfust:	Enthalpy of fusion at a given temperature
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume