Pentane, 2-bromo-

Other names:	2-Bromopentane
	2-Pentyl bromide
	NSC 7896
	UN 2343
Inchi:	InChI=1S/C5H11Br/c1-3-4-5(2)6/h5H,3-4H2,1-2H3
InchiKey:	LGAJYTCRJPCZRJ-UHFFFAOYSA-N
Formula:	C5H11Br
SMILES:	CCCC(C)Br
Mol. weight [g/mol]:	151.04
CAS:	107-81-3

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	38.50	kJ/mol	NIST Webbook
log10ws	-2.46		Crippen Method
logp	2.570		Crippen Method
mcvol	98.810	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	786.00		NIST Webbook
ripol	976.00		NIST Webbook
ripol	984.00		NIST Webbook
ripol	999.00		NIST Webbook
ripol	986.00		NIST Webbook
tb	379.52	K	Joback Method
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	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
cpg	212.94	J/mol×K	568.83	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
dvisc	0.0003481	Pa×s	379.52	Joback Method
hvapt	37.50	kJ/mol	367.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.48220e+01
Coeff. B	-3.57127e+03
Coeff. C	-4.00030e+01
Temperature range (K), min.	285.71
Temperature range (K), max.	415.51

Sources

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=C107813&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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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