

Pentane, 1,4-dibromo-

Other names:	1,4-Dibromopentane
Inchi:	InChI=1S/C5H10Br2/c1-5(7)3-2-4-6/h5H,2-4H2,1H3
InchiKey:	CNBFRBXEGGRSPL-UHFFFAOYSA-N
Formula:	C5H10Br2
SMILES:	CC(Br)CCCB
Mol. weight [g/mol]:	229.94
CAS:	626-87-9

Physical Properties

Property code	Value	Unit	Source
gf	17.42	kJ/mol	Joback Method
hf	-99.15	kJ/mol	Joback Method
hfl	-173.20	kJ/mol	NIST Webbook
hfus	15.75	kJ/mol	Joback Method
hvap	39.21	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.945		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	4151.61	kPa	Joback Method
rinpol	1103.00		NIST Webbook
rinpol	1113.00		NIST Webbook
tb	445.68	K	Joback Method
tc	654.58	K	Joback Method
tf	250.71	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.09	J/molxK	445.68	Joback Method
cpg	204.52	J/molxK	480.50	Joback Method
cpg	213.39	J/molxK	515.31	Joback Method
cpg	221.74	J/molxK	550.13	Joback Method
cpg	229.60	J/molxK	584.95	Joback Method

cpg	237.00	J/molxK	619.76	Joback Method
cpg	243.97	J/molxK	654.58	Joback Method
dvisc	0.0043813	Paxs	250.71	Joback Method
dvisc	0.0023206	Paxs	283.20	Joback Method
dvisc	0.0014009	Paxs	315.70	Joback Method
dvisc	0.0009293	Paxs	348.19	Joback Method
dvisc	0.0006612	Paxs	380.69	Joback Method
dvisc	0.0004963	Paxs	413.19	Joback Method
dvisc	0.0003884	Paxs	445.68	Joback Method
hvapt	51.80	kJ/mol	450.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	371.70	K	3.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.65631e+01
Coeff. B	-4.65211e+03
Coeff. C	-7.26860e+01
Temperature range (K), min.	358.52
Temperature range (K), max.	486.15

Sources

The Yaws Handbook of Vapor

Pressure:
Crippen Method:

Crippen Method:

Joback Method:

McGowan Method:

NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

https://www.chemeo.com/doc/models/crippen_log10ws

https://en.wikipedia.org/wiki/Joback_method

<http://link.springer.com/article/10.1007/BF02311772>

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C626879&Units=SI>

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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