Tetradecane, 1-bromo-

Other names:	1-Bromotetradecane
	1-Tetradecyl bromide
	Myristyl bromide
	Tetradecyl bromide
	n-Tetradecyl bromide
	n-Tetradecyl-1-bromide
Inchi:	InChI=1S/C14H29Br/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15/h2-14H2,1H3
InchiKey:	KOFZTCSTGIWCQG-UHFFFAOYSA-N
Formula:	C14H29Br
SMILES:	CCCCCCCCCCCCCCBr
Mol. weight [g/mol]:	277.28
CAS:	112-71-0

Physical Properties

Property code	Value	Unit	Source
gf	81.32	kJ/mol	Joback Method
hf	-305.96	kJ/mol	Joback Method
hfus	37.30	kJ/mol	Joback Method
hvap	53.19	kJ/mol	Joback Method
log10ws	-6.11		Crippen Method
logp	6.082		Crippen Method
mcvol	225.620	ml/mol	McGowan Method
pc	1609.00	kPa	Joback Method
rinpol	1753.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1758.00		NIST Webbook
ripol	2007.00		NIST Webbook
ripol	2013.00		NIST Webbook
ripol	2037.00		NIST Webbook
tb	580.20	K	NIST Webbook
tc	757.97	K	Joback Method
tf	307.34	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.54	J/mol×K	585.88	Joback Method
cpg	596.52	J/mol×K	643.24	Joback Method
cpg	627.57	J/mol×K	700.61	Joback Method
cpg	642.07	J/mol×K	729.29	Joback Method
cpg	655.92	J/mol×K	757.97	Joback Method
cpg	579.91	J/mol×K	614.56	Joback Method
cpg	612.39	J/mol×K	671.93	Joback Method
dvisc	0.0033625	Pa×s	307.34	Joback Method
dvisc	0.0007931	Pa×s	400.19	Joback Method
dvisc	0.0004825	Pa×s	446.61	Joback Method
dvisc	0.0003223	Pa×s	493.03	Joback Method
dvisc	0.0001743	Pa×s	585.88	Joback Method
dvisc	0.0002308	Pa×s	539.46	Joback Method
dvisc	0.0014854	Pa×s	353.76	Joback Method
hvapt	67.10	kJ/mol	541.00	NIST Webbook
rhol	932.90	kg/m3	393.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	949.80	kg/m3	373.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	945.60	kg/m3	378.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	941.30	kg/m3	383.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

rhol	937.10	kg/m3	388.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	954.00	kg/m3	368.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	928.60	kg/m3	398.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	924.40	kg/m3	403.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	920.10	kg/m3	408.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	915.90	kg/m3	413.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	911.60	kg/m3	418.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	907.40	kg/m3	423.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	958.20	kg/m3	363.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

rhol	962.40	kg/m3	358.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	966.60	kg/m3	353.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	970.80	kg/m3	348.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	974.90	kg/m3	343.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	979.10	kg/m3	338.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	983.30	kg/m3	333.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	987.40	kg/m3	328.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	991.60	kg/m3	323.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

rhol	999.80	kg/m3	313.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	1003.90	kg/m3	308.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	1008.10	kg/m3	303.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	1012.20	kg/m3	298.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes
rhol	995.70	kg/m3	318.15	Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	449.70	K	2.70	NIST Webbook
tbrp	448.00	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54925e+01

Coeff. B	-5.19535e+03
Coeff. C	-1.02432e+02
Temperature range (K), min.	444.12
Temperature range (K), max.	612.73

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C112710&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
Isobaric heat capacity, isothermal compressibility and fluctuational properties of 1-bromoalkanes:	https://www.doi.org/10.1007/s10765-016-2064-y
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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rhol:	Liquid Density
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

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