Hexadecane, 1-bromo-

Other names:	1-Bromohexadecane
	1-Hexadecyl bromide
	CETYL BROMIDE
	Hexadecyl bromide
	N-HEXADECYL BROMIDE
	n-Hexadecyl-1-bromide
Inchi:	InChI=1S/C16H33Br/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h2-16H2,1H3
InchiKey:	HNTGIJLWHDPAFN-UHFFFAOYSA-N
Formula:	C16H33Br
SMILES:	CCCCCCCCCCCCCCCCBr
Mol. weight [g/mol]:	305.34
CAS:	112-82-3

Physical Properties

Property code	Value	Unit	Source
chl	-10567.80 ± 1.70	kJ/mol	NIST Webbook
gf	98.16	kJ/mol	Joback Method
hf	-350.10 ± 3.20	kJ/mol	NIST Webbook
hfl	-444.50 ± 2.80	kJ/mol	NIST Webbook
hfus	42.48	kJ/mol	Joback Method
hvap	94.40	kJ/mol	NIST Webbook
hvap	94.40 ± 1.50	kJ/mol	NIST Webbook
hvap	94.40 ± 1.50	kJ/mol	NIST Webbook
hvap	94.40 ± 1.50	kJ/mol	NIST Webbook
log10ws	-6.95		Crippen Method
logp	6.863		Crippen Method
mcvol	253.800	ml/mol	McGowan Method
pc	1387.11	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
ripol	2237.00		NIST Webbook
ripol	2258.00		NIST Webbook
ripol	2220.00		NIST Webbook
ripol	2258.00		NIST Webbook
ripol	2237.00		NIST Webbook

tb	609.20	K	NIST Webbook
tb	463.15	K	KDB
tc	802.23	K	Joback Method
tf	287.35	K	Fabrication and properties of poly(polyethylene glycol n-alkyl ether vinyl ether)s as polymeric phase change materials
tf	288.15 ± 1.50	K	NIST Webbook
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.67	J/mol×K	631.64	Joback Method
cpg	688.95	J/mol×K	660.07	Joback Method
cpg	706.44	J/mol×K	688.50	Joback Method
cpg	723.15	J/mol×K	716.93	Joback Method
cpg	739.12	J/mol×K	745.36	Joback Method
cpg	754.38	J/mol×K	773.79	Joback Method
cpg	768.96	J/mol×K	802.23	Joback Method
dvisc	0.0028764	Pa×s	329.88	Joback Method
dvisc	0.0012382	Pa×s	380.17	Joback Method
dvisc	0.0006491	Pa×s	430.47	Joback Method
dvisc	0.0003895	Pa×s	480.76	Joback Method
dvisc	0.0002574	Pa×s	531.05	Joback Method
dvisc	0.0001828	Pa×s	581.35	Joback Method
dvisc	0.0001371	Pa×s	631.64	Joback Method
hvapt	71.90	kJ/mol	567.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	463.20	K	1.50	NIST Webbook
tbrp	463.00	K	1.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55101e+01
Coeff. B	-5.43178e+03
Coeff. C	-1.10494e+02
Temperature range (K), min.	467.32
Temperature range (K), max.	643.09

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.20080e+02
Coeff. B	-1.45997e+04
Coeff. C	-1.45223e+01
Coeff. D	4.37035e-06
Temperature range (K), min.	461.15
Temperature range (K), max.	673.15

Sources

KDB: https://www.cheric.org/files/research/kdb/mol/mol1655.mol

Fabrication and properties of poly(polyethylene glycol n-alkyl ether vinyl ether)s as polymeric phase change materials: https://www.doi.org/10.1016/j.tca.2016.04.007

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1655

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C112823&Units=SI

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

Legend

chl:	Standard liquid enthalpy of combustion
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
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