Heptadecane, 1-bromo-

Other names:	1-Bromoheptadecane
	Heptadecyl bromide
	n-Heptadecyl bromide
Inchi:	InChI=1S/C17H35Br/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18/h2-17H2,1H3
InchiKey:	HHSDZLLPIXMEIU-UHFFFAOYSA-N
Formula:	C17H35Br
SMILES:	CCCCCCCCCCCCCCCCCBr
Mol. weight [g/mol]:	319.36
CAS:	3508-00-7

Physical Properties

Property code	Value	Unit	Source
gf	106.58	kJ/mol	Joback Method
hf	-367.88	kJ/mol	Joback Method
hfus	45.07	kJ/mol	Joback Method
hvap	59.87	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	7.253		Crippen Method
mcvol	267.890	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2059.00		NIST Webbook
tb	654.52	K	Joback Method
tc	824.86	K	Joback Method
tf	341.15	K	Joback Method
vc	1.050	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.21	J/mol×K	824.86	Joback Method
cpg	726.75	J/mol×K	654.52	Joback Method
cpg	745.45	J/mol×K	682.91	Joback Method
cpg	763.33	J/mol×K	711.30	Joback Method
cpg	780.41	J/mol×K	739.69	Joback Method

cpg	796.73	J/mol×K	768.08	Joback Method
cpg	812.32	J/mol×K	796.47	Joback Method
dvisc	0.0001208	Pa×s	654.52	Joback Method
dvisc	0.0026326	Pa×s	341.15	Joback Method
dvisc	0.0011200	Pa×s	393.38	Joback Method
dvisc	0.0005822	Pa×s	445.61	Joback Method
dvisc	0.0003472	Pa×s	497.83	Joback Method
dvisc	0.0002284	Pa×s	550.06	Joback Method
dvisc	0.0001616	Pa×s	602.29	Joback Method
hvapt	71.60	kJ/mol	572.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54558e+01
Coeff. B	-5.51533e+03
Coeff. C	-1.14108e+02
Temperature range (K), min.	477.72
Temperature range (K), max.	657.80

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3508007&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

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