Pentadecane, 1-bromo-

Other names:	1-Bromopentadecane
	Pentadecyl bromide
	n-Pentadecyl bromide
Inchi:	InChI=1S/C15H31Br/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16/h2-15H2,1H3
InchiKey:	JKOTZBXSNOGCIF-UHFFFAOYSA-N
Formula:	C15H31Br
SMILES:	CCCCCCCCCCCCCCCBr
Mol. weight [g/mol]:	291.31
CAS:	629-72-1

Physical Properties

Property code	Value	Unit	Source
gf	89.74	kJ/mol	Joback Method
hf	-326.60	kJ/mol	Joback Method
hfus	39.89	kJ/mol	Joback Method
hvap	55.42	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	6.473		Crippen Method
mcvol	239.710	ml/mol	McGowan Method
pc	1491.89	kPa	Joback Method
rinpol	1854.00		NIST Webbook
rinpol	1854.00		NIST Webbook
tb	595.20	K	NIST Webbook
tc	779.95	K	Joback Method
tf	291.70 ± 0.30	K	NIST Webbook
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.85	J/mol×K	779.95	Joback Method
cpg	615.90	J/mol×K	608.76	Joback Method
cpg	633.75	J/mol×K	637.29	Joback Method
cpg	650.82	J/mol×K	665.82	Joback Method

cpg	667.13	J/mol×K	694.35	Joback Method
cpg	682.72	J/mol×K	722.88	Joback Method
cpg	697.62	J/mol×K	751.41	Joback Method
dvisc	0.0001549	Pa×s	608.76	Joback Method
dvisc	0.0031216	Pa×s	318.61	Joback Method
dvisc	0.0013607	Pa×s	366.97	Joback Method
dvisc	0.0007196	Pa×s	415.33	Joback Method
dvisc	0.0004347	Pa×s	463.69	Joback Method
dvisc	0.0002888	Pa×s	512.04	Joback Method
dvisc	0.0002059	Pa×s	560.40	Joback Method
hvapt	69.50	kJ/mol	555.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	432.70	K	0.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55018e+01
Coeff. B	-5.31764e+03
Coeff. C	-1.06602e+02
Temperature range (K), min.	456.12
Temperature range (K), max.	628.43

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C629721&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

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
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