

6-BROMO-1-HEXENE

Other names:	1-Bromo-5-hexene 5-Hexen-1-yl bromide 5-Hexenyl bromide 6-Bromohexene 6-bromohex-1-ene
Inchi:	InChI=1S/C6H11Br/c1-2-3-4-5-6-7/h2H,1,3-6H2
InchiKey:	RIMXEJYJXDBLIE-UHFFFAOYSA-N
Formula:	C6H11Br
SMILES:	C=CCCCCBr
Mol. weight [g/mol]:	163.06
CAS:	2695-47-8

Physical Properties

Property code	Value	Unit	Source
af	0.4017		Cheméo Relay (1.0)
gf	101.80	kJ/mol	Joback Method
hf	-23.85	kJ/mol	Cheméo Relay (1.0)
hfus	15.30	kJ/mol	Joback Method
hvap	45.64	kJ/mol	Cheméo Relay (1.0)
ie	9.65	eV	Cheméo Relay (1.0)
log10ws	-3.09		Cheméo Relay (1.0)
logp	2.738		Crippen Method
mcvol	108.600	ml/mol	McGowan Method
pc	3530.46	kPa	Joback Method
tb	422.41	K	Cheméo Relay (1.0)
tc	607.21	K	Cheméo Relay (1.0)
tf	186.89	K	Cheméo Relay (1.0)
vc	0.390	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.92	J/mol×K	399.52	Joback Method
cpg	192.94	J/mol×K	430.80	Joback Method

cpg	202.46	J/mol×K	462.09	Joback Method
cpg	211.51	J/mol×K	493.37	Joback Method
cpg	220.11	J/mol×K	524.66	Joback Method
cpg	228.27	J/mol×K	555.94	Joback Method
cpg	236.03	J/mol×K	587.23	Joback Method
dvisc	0.0035539	Pa×s	215.42	Joback Method
dvisc	0.0018857	Pa×s	246.10	Joback Method
dvisc	0.0011515	Pa×s	276.79	Joback Method
dvisc	0.0007759	Pa×s	307.47	Joback Method
dvisc	0.0005616	Pa×s	338.15	Joback Method
dvisc	0.0004290	Pa×s	368.84	Joback Method
dvisc	0.0003415	Pa×s	399.52	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	322.20	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.34468e+01
Coeff. B	-3.38355e+03
Coeff. C	-5.73960e+01
Temperature range (K), min.	314.52
Temperature range (K), max.	473.30

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor
Pressure:
NIST Webbook:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2695478&Units=SI>

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
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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