1-Hexene, 1-bromo-, (E)-

Other names: trans-1-Bromo-1-Hexene
Inchi: InChI=1S/C6H11Br/c1-2-3-4-5-6-7/h5-6H,2-4H2,1H3/b6-5+
InchiKey: FBUZNPORDKVYFD-AATRIKPKSA-N
Formula: C6H11Br
SMILES: CCCCC=CBr
Mol. weight [g/mol]: 163.06
CAS: 13154-13-7

Physical Properties

Property code	Value	Unit	Source
gf	94.18	kJ/mol	Joback Method
hf	-23.62	kJ/mol	Joback Method
hfus	16.78	kJ/mol	Joback Method
hvap	35.34	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	3.085		Crippen Method
mcvol	108.600	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	407.00	K	Joback Method
tc	600.32	K	Joback Method
tf	212.10	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.39	J/mol×K	407.00	Joback Method
cpg	192.73	J/mol×K	439.22	Joback Method
cpg	202.50	J/mol×K	471.44	Joback Method
cpg	211.74	J/mol×K	503.66	Joback Method
cpg	220.47	J/mol×K	535.88	Joback Method
cpg	228.72	J/mol×K	568.10	Joback Method
cpg	236.53	J/mol×K	600.32	Joback Method
dvisc	0.0037427	Pa×s	212.10	Joback Method

dvisc	0.0018371	Pa×s	244.58	Joback Method
dvisc	0.0010655	Pa×s	277.07	Joback Method
dvisc	0.0006929	Pa×s	309.55	Joback Method
dvisc	0.0004889	Pa×s	342.03	Joback Method
dvisc	0.0003665	Pa×s	374.52	Joback Method
dvisc	0.0002877	Pa×s	407.00	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51144e+01
Coeff. B	-3.73656e+03
Coeff. C	-5.60060e+01
Temperature range (K), min.	308.02
Temperature range (K), max.	437.17

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13154137&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

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

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