Heptane, 3-(bromomethyl)-

Other names:	1-Bromo-2-ethylhexane
	2-Ethylhexyl bromide
	3-(Bromomethyl)heptane
	Hexane, 1-bromo-2-ethyl
Inchi:	InChI=1S/C8H17Br/c1-3-5-6-8(4-2)7-9/h8H,3-7H2,1-2H3
InchiKey:	NZWIYPLSXWYKLH-UHFFFAOYSA-N
Formula:	C8H17Br
SMILES:	CCCCC(CC)CBr
Mol. weight [g/mol]:	193.12
CAS:	18908-66-2

Physical Properties

Property code	Value	Unit	Source
gf	28.36	kJ/mol	Joback Method
hf	-187.40	kJ/mol	Joback Method
hfus	18.24	kJ/mol	Joback Method
hvap	39.45	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.598		Crippen Method
mcvol	141.080	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
tb	448.16	K	Joback Method
tc	633.14	K	Joback Method
tf	224.72	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	277.18	J/mol×K	448.16	Joback Method
cpg	338.14	J/mol×K	602.31	Joback Method
cpg	327.07	J/mol×K	571.48	Joback Method
cpg	315.46	J/mol×K	540.65	Joback Method
cpg	303.29	J/mol×K	509.82	Joback Method

cpg	290.54	J/mol×K	478.99	Joback Method
cpg	348.69	J/mol×K	633.14	Joback Method
dvisc	0.0002948	Pa×s	448.16	Joback Method
dvisc	0.0003902	Pa×s	410.92	Joback Method
dvisc	0.0005461	Pa×s	373.68	Joback Method
dvisc	0.0008234	Pa×s	336.44	Joback Method
dvisc	0.0013751	Pa×s	299.20	Joback Method
dvisc	0.0026570	Pa×s	261.96	Joback Method
dvisc	0.0063866	Pa×s	224.72	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	349.20	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47604e+01
Coeff. B	-4.02200e+03
Coeff. C	-6.84600e+01
Temperature range (K), min.	346.36
Temperature range (K), max.	494.12

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18908662&Units=SI

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

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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume