4-Bromoheptane

Other names: Heptane, 4-bromo-
Inchi: InChI=1S/C7H15Br/c1-3-5-7(8)6-4-2/h7H,3-6H2,1-2H3
InchiKey: BNUTXEKPXPZAIT-UHFFFAOYSA-N
Formula: C7H15Br
SMILES: CCCC(Br)CCC
Mol. weight [g/mol]: 179.10
CAS: 998-93-6

Physical Properties

Property code	Value	Unit	Source
gf	19.94	kJ/mol	Joback Method
hf	-166.76	kJ/mol	Joback Method
hfus	15.65	kJ/mol	Joback Method
hvap	37.22	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.350		Crippen Method
mcvol	126.990	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	1025.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	1039.00		NIST Webbook
ripol	1138.00		NIST Webbook
ripol	1142.00		NIST Webbook
ripol	1164.00		NIST Webbook
tb	425.28	K	Joback Method
tc	611.91	K	Joback Method
tf	213.45	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	236.30	J/mol×K	425.28	Joback Method
cpg	248.56	J/mol×K	456.38	Joback Method

cpg	260.26	J/mol×K	487.49	Joback Method
cpg	271.43	J/mol×K	518.59	Joback Method
cpg	282.08	J/mol×K	549.70	Joback Method
cpg	292.23	J/mol×K	580.80	Joback Method
cpg	301.90	J/mol×K	611.91	Joback Method
dvisc	0.0064391	Pa×s	213.45	Joback Method
dvisc	0.0027270	Pa×s	248.75	Joback Method
dvisc	0.0014299	Pa×s	284.06	Joback Method
dvisc	0.0008648	Pa×s	319.37	Joback Method
dvisc	0.0005781	Pa×s	354.67	Joback Method
dvisc	0.0004157	Pa×s	389.98	Joback Method
dvisc	0.0003157	Pa×s	425.28	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.80	K	9.60	NIST Webbook
tbrp	333.20	K	2.40	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.45289e+01
Coeff. B	-3.78072e+03
Coeff. C	-6.18440e+01
Temperature range (K), min.	327.32
Temperature range (K), max.	472.02

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=C998936&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
rinpol:	Non-polar retention indices
ripol:	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