Heptane, 2-bromo-

Other names: 2-Bromoheptane
2-Heptyl bromide
Inchi: InChI=1S/C7H15Br/c1-3-4-5-6-7(2)8/h7H,3-6H2,1-2H3
InchiKey: HLAUCEOFCOXKNF-UHFFFAOYSA-N
Formula: C7H15Br
SMILES: CCCCCC(C)Br
Mol. weight [g/mol]: 179.10
CAS: 1974-04-5

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	1037.00		NIST Webbook
rinpol	1047.00		NIST Webbook
rinpol	1026.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	1037.00		NIST Webbook
rinpol	986.00		NIST Webbook
ripol	1173.00		NIST Webbook
ripol	1173.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1185.00		NIST Webbook
ripol	1175.00		NIST Webbook
tb	439.00 ± 3.00	K	NIST Webbook
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	301.90	J/mol×K	611.91	Joback Method
cpg	292.23	J/mol×K	580.80	Joback Method
cpg	282.08	J/mol×K	549.70	Joback Method
cpg	271.43	J/mol×K	518.59	Joback Method
cpg	260.26	J/mol×K	487.49	Joback Method
cpg	248.56	J/mol×K	456.38	Joback Method
cpg	236.30	J/mol×K	425.28	Joback Method
dvisc	0.0064391	Pa×s	213.45	Joback Method
dvisc	0.0003157	Pa×s	425.28	Joback Method
dvisc	0.0004157	Pa×s	389.98	Joback Method
dvisc	0.0005781	Pa×s	354.67	Joback Method
dvisc	0.0008648	Pa×s	319.37	Joback Method
dvisc	0.0014299	Pa×s	284.06	Joback Method
dvisc	0.0027270	Pa×s	248.75	Joback Method
hvapt	45.00	kJ/mol	386.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	338.20	K	2.80	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54004e+01
Coeff. B	-4.05153e+03
Coeff. C	-6.32340e+01
Temperature range (K), min.	320.15
Temperature range (K), max.	464.82

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1974045&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

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
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