Hexane, 3-bromo-

Other names: 3-Bromohexane
Inchi: InChI=1S/C6H13Br/c1-3-5-6(7)4-2/h6H,3-5H2,1-2H3
InchiKey: IOZOJWNUKLCDML-UHFFFAOYSA-N
Formula: C6H13Br
SMILES: CCCC(Br)CC
Mol. weight [g/mol]: 165.07
CAS: 3377-87-5

Physical Properties

Property code	Value	Unit	Source
gf	11.52	kJ/mol	Joback Method
hf	-146.12	kJ/mol	Joback Method
hfus	13.06	kJ/mol	Joback Method
hvap	35.00	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.960		Crippen Method
mcvol	112.900	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
rinpol	943.00		NIST Webbook
rinpol	943.00		NIST Webbook
rinpol	951.00		NIST Webbook
rinpol	953.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1059.00		NIST Webbook
ripol	1073.00		NIST Webbook
tb	415.00	K	NIST Webbook
tb	415.00 ± 2.00	K	NIST Webbook
tc	590.50	K	Joback Method
tf	202.18	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	197.64	J/mol×K	402.40	Joback Method
cpg	247.93	J/mol×K	559.15	Joback Method
cpg	238.81	J/mol×K	527.80	Joback Method
cpg	229.23	J/mol×K	496.45	Joback Method
cpg	219.19	J/mol×K	465.10	Joback Method
cpg	208.66	J/mol×K	433.75	Joback Method
cpg	256.62	J/mol×K	590.50	Joback Method
dvisc	0.0003340	Pa×s	402.40	Joback Method
dvisc	0.0004371	Pa×s	369.03	Joback Method
dvisc	0.0006036	Pa×s	335.66	Joback Method
dvisc	0.0008951	Pa×s	302.29	Joback Method
dvisc	0.0014638	Pa×s	268.92	Joback Method
dvisc	0.0027514	Pa×s	235.55	Joback Method
dvisc	0.0063698	Pa×s	202.18	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53025e+01
Coeff. B	-3.83170e+03
Coeff. C	-5.63670e+01
Temperature range (K), min.	311.56
Temperature range (K), max.	439.88

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3377875&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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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