Hexane, 2-bromo-

Other names: (dl) 2-bromohexane
2-Bromohexane
Inchi: InChI=1S/C6H13Br/c1-3-4-5-6(2)7/h6H,3-5H2,1-2H3
InchiKey: NEBYCXAKZCQWAW-UHFFFAOYSA-N
Formula: C6H13Br
SMILES: CCCCC(C)Br
Mol. weight [g/mol]: 165.07
CAS: 3377-86-4

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	952.00		NIST Webbook
rinpol	934.00		NIST Webbook
rinpol	941.00		NIST Webbook
ripol	1069.00		NIST Webbook
ripol	1077.00		NIST Webbook
ripol	1091.00		NIST Webbook
tb	402.40	K	Joback Method
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	256.62	J/mol×K	590.50	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	197.64	J/mol×K	402.40	Joback Method
dvisc	0.0063698	Pa×s	202.18	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
hvapt	43.80	kJ/mol	359.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50246e+01
Coeff. B	-3.78078e+03
Coeff. C	-5.70900e+01
Temperature range (K), min.	313.64
Temperature range (K), max.	446.33

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3377864&Units=SI

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