1-Bromo-4-methylhexane

Inchi: InChI=1S/C7H15Br/c1-3-7(2)5-4-6-8/h7H,3-6H2,1-2H3
InchiKey: QIXNVYCYRYRCAK-UHFFFAOYSA-N
Formula: C7H15Br
SMILES: CCC(C)CCCBr
Mol. weight [g/mol]: 179.10
CAS: ---

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	-2.94		Crippen Method
logp	3.208		Crippen Method
mcvol	126.990	ml/mol	McGowan Method
pc	3042.32	kPa	Joback Method
rinpol	1013.00		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	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	301.90	J/mol×K	611.91	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
dvisc	0.0064391	Pa×s	213.45	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52627e+01
Coeff. B	-4.03730e+03
Coeff. C	-6.40400e+01
Temperature range (K), min.	333.64
Temperature range (K), max.	469.75

Sources

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=R412578&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

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