Pentane, 1-bromo-3-methyl-

Other names: 1-Bromo-3-methylpentane
BrCH2CH2CH(CH3)C2H5
Inchi: InChI=1S/C6H13Br/c1-3-6(2)4-5-7/h6H,3-5H2,1-2H3
InchiKey: MDCCBJLCTOTLKM-UHFFFAOYSA-N
Formula: C6H13Br
SMILES: CCC(C)CCBr
Mol. weight [g/mol]: 165.07
CAS: 51116-73-5

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	-2.52		Crippen Method
logp	2.817		Crippen Method
mcvol	112.900	ml/mol	McGowan Method
pc	3392.03	kPa	Joback Method
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	197.64	J/mol×K	402.40	Joback Method
cpg	208.66	J/mol×K	433.75	Joback Method
cpg	219.19	J/mol×K	465.10	Joback Method
cpg	229.23	J/mol×K	496.45	Joback Method
cpg	238.81	J/mol×K	527.80	Joback Method
cpg	247.93	J/mol×K	559.15	Joback Method
cpg	256.62	J/mol×K	590.50	Joback Method

dvisc	0.0063698	Pa×s	202.18	Joback Method
dvisc	0.0027514	Pa×s	235.55	Joback Method
dvisc	0.0014638	Pa×s	268.92	Joback Method
dvisc	0.0008951	Pa×s	302.29	Joback Method
dvisc	0.0006036	Pa×s	335.66	Joback Method
dvisc	0.0004371	Pa×s	369.03	Joback Method
dvisc	0.0003340	Pa×s	402.40	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54440e+01
Coeff. B	-3.92081e+03
Coeff. C	-5.82300e+01
Temperature range (K), min.	316.92
Temperature range (K), max.	445.18

Sources

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=C51116735&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

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

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