Pentane, 2-bromo-4-methyl-

Other names: 2-Bromo-4-methylpentane
Inchi: InChI=1S/C6H13Br/c1-5(2)4-6(3)7/h5-6H,4H2,1-3H3
InchiKey: IUXIOXCOPJFKMQ-UHFFFAOYSA-N
Formula: C6H13Br
SMILES: CC(C)CC(C)Br
Mol. weight [g/mol]: 165.07
CAS: 30310-22-6

Physical Properties

Property code	Value	Unit	Source
gf	9.08	kJ/mol	Joback Method
hf	-151.40	kJ/mol	Joback Method
hfus	9.53	kJ/mol	Joback Method
hvap	34.61	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.816		Crippen Method
mcvol	112.900	ml/mol	McGowan Method
pc	3423.86	kPa	Joback Method
rinpol	917.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	935.00		NIST Webbook
rinpol	940.00		NIST Webbook
rinpol	950.00		NIST Webbook
rinpol	935.00		NIST Webbook
ripol	1003.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1037.00		NIST Webbook
tb	404.50 ± 1.50	K	NIST Webbook
tc	594.59	K	Joback Method
tf	178.60 ± 1.50	K	NIST Webbook
tf	179.15 ± 1.50	K	NIST Webbook
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.33	J/mol×K	594.59	Joback Method
cpg	197.63	J/mol×K	401.96	Joback Method
cpg	209.01	J/mol×K	434.06	Joback Method
cpg	219.87	J/mol×K	466.17	Joback Method
cpg	230.21	J/mol×K	498.27	Joback Method
cpg	240.06	J/mol×K	530.38	Joback Method
cpg	249.42	J/mol×K	562.48	Joback Method
dvisc	0.0003219	Pa×s	401.96	Joback Method
dvisc	0.0109622	Pa×s	187.18	Joback Method
dvisc	0.0037982	Pa×s	222.98	Joback Method
dvisc	0.0017644	Pa×s	258.77	Joback Method
dvisc	0.0009876	Pa×s	294.57	Joback Method
dvisc	0.0006268	Pa×s	330.37	Joback Method
dvisc	0.0004348	Pa×s	366.16	Joback Method
hvapt	29.30	kJ/mol	381.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.53110e+01
Coeff. B	-3.75310e+03
Coeff. C	-5.35040e+01
Temperature range (K), min.	303.32
Temperature range (K), max.	428.83

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30310226&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
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