Pentane, 3-bromo-3-methyl-

Other names: 3-Bromo-3-methylpentane
Inchi: InChI=1S/C6H13Br/c1-4-6(3,7)5-2/h4-5H2,1-3H3
InchiKey: ZRPQYKLJSOLRPZ-UHFFFAOYSA-N
Formula: C6H13Br
SMILES: CCC(C)(Br)CC
Mol. weight [g/mol]: 165.07
CAS: 25346-31-0

Physical Properties

Property code	Value	Unit	Source
gf	16.80	kJ/mol	Joback Method
hf	-149.59	kJ/mol	Joback Method
hfus	9.17	kJ/mol	Joback Method
hvap	34.09	kJ/mol	Joback Method
log10ws	-2.88		Crippen Method
logp	2.960		Crippen Method
mcvol	112.900	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
rinpol	876.00		NIST Webbook
rinpol	876.00		NIST Webbook
rinpol	929.00		NIST Webbook
rinpol	916.00		NIST Webbook
rinpol	944.00		NIST Webbook
ripol	1037.00		NIST Webbook
ripol	1047.00		NIST Webbook
ripol	1059.00		NIST Webbook
tb	399.61	K	Joback Method
tc	595.92	K	Joback Method
tf	180.95 ± 0.50	K	NIST Webbook
vc	0.422	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	199.46	J/mol×K	399.61	Joback Method
cpg	211.57	J/mol×K	432.33	Joback Method
cpg	222.97	J/mol×K	465.05	Joback Method
cpg	233.70	J/mol×K	497.77	Joback Method
cpg	243.79	J/mol×K	530.48	Joback Method
cpg	253.28	J/mol×K	563.20	Joback Method
cpg	262.20	J/mol×K	595.92	Joback Method
dvisc	0.0067171	Pa×s	219.60	Joback Method
dvisc	0.0031204	Pa×s	249.60	Joback Method
dvisc	0.0017088	Pa×s	279.60	Joback Method
dvisc	0.0010517	Pa×s	309.61	Joback Method
dvisc	0.0007052	Pa×s	339.61	Joback Method
dvisc	0.0005045	Pa×s	369.61	Joback Method
dvisc	0.0003796	Pa×s	399.61	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37764e+01
Coeff. B	-3.36269e+03
Coeff. C	-5.32260e+01
Temperature range (K), min.	302.52
Temperature range (K), max.	450.47

Sources

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=C25346310&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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