1-Bromo-3,3-dimethylbutane

Other names:	BrCH2CH2C(CH3)3
	Butane, 1-bromo-3,3-dimethyl-
Inchi:	InChI=1S/C6H13Br/c1-6(2,3)4-5-7/h4-5H2,1-3H3
InchiKey:	ROKZAMCDHKVZIQ-UHFFFAOYSA-N
Formula:	C6H13Br
SMILES:	CC(C)(C)CCBr
Mol. weight [g/mol]:	165.07
CAS:	1647-23-0

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	-2.52		Crippen Method
logp	2.817		Crippen Method
mcvol	112.900	ml/mol	McGowan Method
pc	3435.91	kPa	Joback Method
tb	399.61	K	Joback Method
tc	595.92	K	Joback Method
tf	219.60	K	Joback Method
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	1.43741e+01
Coeff. B	-3.56316e+03
Coeff. C	-5.51720e+01
Temperature range (K), min.	308.12
Temperature range (K), max.	448.34

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1647230&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

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