

Hexane, 2-bromo-2-methyl

Other names:	2-Bromo-2-methylhexane
Inchi:	InChI=1S/C7H15Br/c1-4-5-6-7(2,3)8/h4-6H2,1-3H3
InchiKey:	FVGJIAVGOPDNHY-UHFFFAOYSA-N
Formula:	C7H15Br
SMILES:	CCCCC(C)(C)Br
Mol. weight [g/mol]:	179.10
CAS:	---

Physical Properties

Property code	Value	Unit	Source
gf	25.22	kJ/mol	Joback Method
hf	-170.23	kJ/mol	Joback Method
hfus	11.76	kJ/mol	Joback Method
hvap	36.31	kJ/mol	Joback Method
log10ws	-3.30		Crippen Method
logp	3.350		Crippen Method
mcvol	126.990	ml/mol	McGowan Method
pc	3079.57	kPa	Joback Method
rinpol	942.00		NIST Webbook
rinpol	942.00		NIST Webbook
tb	422.49	K	Joback Method
tc	617.07	K	Joback Method
tf	230.87	K	Joback Method
vc	0.478	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	238.41	J/molxK	422.49	Joback Method
cpg	297.60	J/molxK	584.64	Joback Method
cpg	287.12	J/molxK	552.21	Joback Method
cpg	276.00	J/molxK	519.78	Joback Method
cpg	264.20	J/molxK	487.35	Joback Method
cpg	251.68	J/molxK	454.92	Joback Method

cpg	307.48	J/molxK	617.07	Joback Method
dvisc	0.0003489	Paxs	422.49	Joback Method
dvisc	0.0004659	Paxs	390.55	Joback Method
dvisc	0.0006552	Paxs	358.62	Joback Method
dvisc	0.0009848	Paxs	326.68	Joback Method
dvisc	0.0016169	Paxs	294.74	Joback Method
dvisc	0.0029947	Paxs	262.81	Joback Method
dvisc	0.0065777	Paxs	230.87	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43471e+01
Coeff. B	-3.71705e+03
Coeff. C	-6.12600e+01
Temperature range (K), min.	325.64
Temperature range (K), max.	472.64

Sources

The Yaws Handbook of Vapor

Pressure:

Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=R32428&Units=SI>

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

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