

1-Bromo-2-methylpentane

Other names:	2-methylpentyl bromide
Inchi:	InChI=1S/C6H13Br/c1-3-4-6(2)5-7/h6H,3-5H2,1-2H3
InchiKey:	GSYMWZIKZUHBKV-UHFFFAOYSA-N
Formula:	C6H13Br
SMILES:	CCCC(C)CBr
Mol. weight [g/mol]:	165.07
CAS:	25346-33-2

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
rinpol	946.00		NIST Webbook
rinpol	956.00		NIST Webbook
rinpol	948.00		NIST Webbook
ripol	1104.00		NIST Webbook
ripol	1112.00		NIST Webbook
ripol	1099.00		NIST Webbook
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/molxK	402.40	Joback Method
cpg	208.66	J/molxK	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	Paxs	202.18	Joback Method
dvisc	0.0027514	Paxs	235.55	Joback Method
dvisc	0.0014638	Paxs	268.92	Joback Method
dvisc	0.0008951	Paxs	302.29	Joback Method
dvisc	0.0006036	Paxs	335.66	Joback Method
dvisc	0.0004371	Paxs	369.03	Joback Method
dvisc	0.0003340	Paxs	402.40	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.50345e+01
Coeff. B	-3.78409e+03
Coeff. C	-5.71180e+01
Temperature range (K), min.	313.72
Temperature range (K), max.	446.31

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=C25346332&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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