

2-Methyl-4-bromo-1-butene

Inchi:	InChI=1S/C5H9Br/c1-5(2)3-4-6/h1,3-4H2,2H3
InchiKey:	IZMWJUPSQXIVDN-UHFFFAOYSA-N
Formula:	C5H9Br
SMILES:	C=C(C)CCBr
Mol. weight [g/mol]:	149.03
CAS:	20038-12-4

Physical Properties

Property code	Value	Unit	Source
gf	84.83	kJ/mol	Joback Method
hf	-4.56	kJ/mol	Joback Method
hfus	11.40	kJ/mol	Joback Method
hvap	32.57	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.348		Crippen Method
mcvol	94.510	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	376.52	K	Joback Method
tc	569.33	K	Joback Method
tf	190.19	K	Joback Method
vc	0.359	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.49	J/mol×K	376.52	Joback Method
cpg	156.27	J/mol×K	408.66	Joback Method
cpg	164.60	J/mol×K	440.79	Joback Method
cpg	172.49	J/mol×K	472.93	Joback Method
cpg	179.96	J/mol×K	505.06	Joback Method
cpg	187.04	J/mol×K	537.20	Joback Method
cpg	193.75	J/mol×K	569.33	Joback Method

Sources

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=C20038124&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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