2-Butene, 1-bromo-2-methyl-

Inchi: InChI=1S/C5H9Br/c1-3-5(2)4-6/h3H,4H2,1-2H3/b5-3+
InchiKey: WZEXBDRUCFODAA-HWKANZROSA-N
Formula: C5H9Br
SMILES: CC=C(C)CBr
Mol. weight [g/mol]: 149.03
CAS: 41178-84-1

Physical Properties

Property code	Value	Unit	Source
gf	77.21	kJ/mol	Joback Method
hf	-12.77	kJ/mol	Joback Method
hfus	12.88	kJ/mol	Joback Method
hvap	33.20	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.348		Crippen Method
mcvol	94.510	ml/mol	McGowan Method
pc	4046.64	kPa	Joback Method
tb	384.00	K	Joback Method
tc	582.88	K	Joback Method
tf	186.87	K	Joback Method
vc	0.358	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	146.47	J/mol×K	384.00	Joback Method
cpg	155.60	J/mol×K	417.15	Joback Method
cpg	164.20	J/mol×K	450.29	Joback Method
cpg	172.29	J/mol×K	483.44	Joback Method
cpg	179.91	J/mol×K	516.59	Joback Method
cpg	187.09	J/mol×K	549.73	Joback Method
cpg	193.86	J/mol×K	582.88	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=C41178841&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