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

Physical Properties

Property code	Value	Unit	Source
af	0.3608		Cheméo Relay (1.0)
hf	-14.35	kJ/mol	Cheméo Relay (1.0)
hfus	11.40	kJ/mol	Joback Method
hvap	39.88	kJ/mol	Cheméo Relay (1.0)
ie	9.57	eV	Cheméo Relay (1.0)
log10ws	-2.53		Cheméo Relay (1.0)
logp	2.348		Crippen Method
mcvol	94.510	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	393.69	K	Cheméo Relay (1.0)
tc	573.04	K	Cheméo Relay (1.0)
tf	189.05	K	Cheméo Relay (1.0)
vc	0.334	m3/kmol	Cheméo Relay (1.0)

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20038124&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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