

(E)-1-Bromo-2-butene

Other names:	2-Butene, 1-bromo-, (E)-
Inchi:	InChI=1S/C4H7Br/c1-2-3-4-5/h2-3H,4H2,1H3/b3-2+
InchiKey:	AVMHMVJVHYGDOO-NSCUHMNNSA-N
Formula:	C4H7Br
SMILES:	CC=CCBr
Mol. weight [g/mol]:	135.00
CAS:	29576-14-5

Physical Properties

Property code	Value	Unit	Source
gf	77.34	kJ/mol	Joback Method
hf	17.66	kJ/mol	Joback Method
hfus	11.60	kJ/mol	Joback Method
hvap	30.89	kJ/mol	Joback Method
log10ws	-1.78		Crippen Method
logp	1.957		Crippen Method
mcvol	80.420	ml/mol	McGowan Method
pc	4559.21	kPa	Joback Method
tb	361.24	K	Joback Method
tc	557.14	K	Joback Method
tf	189.56	K	Joback Method
vc	0.301	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.95	J/molxK	361.24	Joback Method
cpg	146.10	J/molxK	524.49	Joback Method
cpg	140.27	J/molxK	491.84	Joback Method
cpg	134.06	J/molxK	459.19	Joback Method
cpg	127.45	J/molxK	426.54	Joback Method
cpg	120.43	J/molxK	393.89	Joback Method
cpg	151.59	J/molxK	557.14	Joback Method
dvisc	0.0002999	Paxs	361.24	Joback Method

dvisc	0.0003758	Paxs	332.63	Joback Method
dvisc	0.0004915	Paxs	304.01	Joback Method
dvisc	0.0006796	Paxs	275.40	Joback Method
dvisc	0.0010129	Paxs	246.79	Joback Method
dvisc	0.0016765	Paxs	218.17	Joback Method
dvisc	0.0032305	Paxs	189.56	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29576145&Units=SI
Crippen Method:	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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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