

2-Bromo-2-butene

Other names:	2-Butene, 2-bromo- 2-bromobut-2-ene
Inchi:	InChI=1S/C4H7Br/c1-3-4(2)5/h3H,1-2H3
InchiKey:	UILZQFGKPHAAOU-UHFFFAOYSA-N
Formula:	C4H7Br
SMILES:	CC=C(C)Br
Mol. weight [g/mol]:	135.00
CAS:	13294-71-8

Physical Properties

Property code	Value	Unit	Source
gf	68.79	kJ/mol	Joback Method
hf	7.87	kJ/mol	Joback Method
hfus	10.29	kJ/mol	Joback Method
hvap	30.97	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.305		Crippen Method
mvol	80.420	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
tb	361.12	K	Joback Method
tc	561.25	K	Joback Method
tf	175.60	K	Joback Method
vc	0.302	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	112.99	J/molxK	361.12	Joback Method
cpg	120.59	J/molxK	394.48	Joback Method
cpg	127.72	J/molxK	427.83	Joback Method
cpg	134.41	J/molxK	461.19	Joback Method
cpg	140.69	J/molxK	494.54	Joback Method
cpg	146.58	J/molxK	527.90	Joback Method
cpg	152.11	J/molxK	561.25	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.53440e+01
Coeff. B	-3.42730e+03
Coeff. C	-4.16890e+01
Temperature range (K), min.	269.32
Temperature range (K), max.	383.86

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=C13294718&Units=SI>

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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