

2-bromo-1-butene

Inchi:	InChI=1S/C4H7Br/c1-3-4(2)5/h2-3H2,1H3
InchiKey:	HQMXRIGBXOFKIU-UHFFFAOYSA-N
Formula:	C4H7Br
SMILES:	C=C(Br)CC
Mol. weight [g/mol]:	135.00
CAS:	23074-36-4

Physical Properties

Property code	Value	Unit	Source
af	0.2461		Cheméo Relay (1.0)
hf	26.40	kJ/mol	Cheméo Relay (1.0)
hfus	8.81	kJ/mol	Joback Method
hvap	27.89	kJ/mol	Cheméo Relay (1.0)
ie	9.25	eV	Cheméo Relay (1.0)
log10ws	-2.31		Cheméo Relay (1.0)
logp	2.305		Crippen Method
mcvol	80.420	ml/mol	McGowan Method
pc	4528.58	kPa	Joback Method
tb	354.11	K	Cheméo Relay (1.0)
tc	531.24	K	Cheméo Relay (1.0)
tf	147.23	K	Cheméo Relay (1.0)
vc	0.300	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.55	J/mol×K	353.64	Joback Method
cpg	121.78	J/mol×K	385.93	Joback Method
cpg	128.62	J/mol×K	418.22	Joback Method
cpg	135.09	J/mol×K	450.50	Joback Method
cpg	141.21	J/mol×K	482.79	Joback Method
cpg	146.99	J/mol×K	515.08	Joback Method
cpg	152.46	J/mol×K	547.37	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.38555e+01
Coeff. B	-2.95292e+03
Coeff. C	-4.15210e+01
Temperature range (K), min.	259.16
Temperature range (K), max.	387.13

Sources

The Yaws Handbook of Vapor Pressure:
Joback Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
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>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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
pvap: Vapor pressure

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

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