

1-Butene, 3-bromo-

Other names:	3-Bromo-1-butene
Inchi:	InChI=1S/C4H7Br/c1-3-4(2)5/h3-4H,1H2,2H3
InchiKey:	XOTGLEGIDHZTIM-UHFFFAOYSA-N
Formula:	C4H7Br
SMILES:	C=CC(C)Br
Mol. weight [g/mol]:	135.00
CAS:	22037-73-6

Physical Properties

Property code	Value	Unit	Source
gf	82.52	kJ/mol	Joback Method
hf	20.59	kJ/mol	Joback Method
hfus	6.60	kJ/mol	Joback Method
hvap	29.88	kJ/mol	Joback Method
log10ws	-1.89		Crippen Method
logp	1.956		Crippen Method
mcvol	80.420	ml/mol	McGowan Method
pc	4546.92	kPa	Joback Method
tb	353.32	K	Joback Method
tc	547.79	K	Joback Method
tf	177.88	K	Joback Method
vc	0.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	114.39	J/mol×K	353.32	Joback Method
cpg	147.59	J/mol×K	515.38	Joback Method
cpg	141.68	J/mol×K	482.96	Joback Method
cpg	135.42	J/mol×K	450.55	Joback Method
cpg	128.80	J/mol×K	418.14	Joback Method
cpg	121.79	J/mol×K	385.73	Joback Method
cpg	153.18	J/mol×K	547.79	Joback Method
dvisc	0.0003442	Pa×s	353.32	Joback Method

dvisc	0.0004380	Pa×s	324.08	Joback Method
dvisc	0.0005848	Pa×s	294.84	Joback Method
dvisc	0.0008321	Pa×s	265.60	Joback Method
dvisc	0.0012920	Pa×s	236.36	Joback Method
dvisc	0.0022712	Pa×s	207.12	Joback Method
dvisc	0.0048063	Pa×s	177.88	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.56399e+01
Coeff. B	-2.94921e+03
Coeff. C	-9.36450e+01
Temperature range (K), min.	285.75
Temperature range (K), max.	401.88

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22037736&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp _g :	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g _f :	Standard Gibbs free energy of formation
h _f :	Enthalpy of formation at standard conditions
h _{fus} :	Enthalpy of fusion at standard conditions
h _{vap} :	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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