

Butane, 1,3-dibromo-3-methyl-

Other names:	1,3-Dibromo-3-methylbutane
Inchi:	InChI=1S/C5H10Br2/c1-5(2,7)3-4-6/h3-4H2,1-2H3
InchiKey:	XMJFMQSXQQUJTQ-UHFFFAOYSA-N
Formula:	C5H10Br2
SMILES:	CC(C)(Br)CCBr
Mol. weight [g/mol]:	229.94
CAS:	24443-15-0

Physical Properties

Property code	Value	Unit	Source
gf	22.70	kJ/mol	Joback Method
hf	-102.62	kJ/mol	Joback Method
hfus	11.86	kJ/mol	Joback Method
hvap	38.30	kJ/mol	Joback Method
log10ws	-2.89		Crippen Method
logp	2.945		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	4211.09	kPa	Joback Method
tb	442.89	K	Joback Method
tc	661.07	K	Joback Method
tf	268.13	K	Joback Method
vc	0.428	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	197.85	J/molxK	442.89	Joback Method
cpg	208.11	J/molxK	479.25	Joback Method
cpg	217.61	J/molxK	515.62	Joback Method
cpg	226.38	J/molxK	551.98	Joback Method
cpg	234.49	J/molxK	588.34	Joback Method
cpg	242.00	J/molxK	624.70	Joback Method
cpg	248.94	J/molxK	661.07	Joback Method
dvisc	0.0043647	Paxs	268.13	Joback Method

dvisc	0.0024400	Paxs	297.26	Joback Method
dvisc	0.0015133	Paxs	326.38	Joback Method
dvisc	0.0010149	Paxs	355.51	Joback Method
dvisc	0.0007231	Paxs	384.64	Joback Method
dvisc	0.0005404	Paxs	413.76	Joback Method
dvisc	0.0004197	Paxs	442.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	347.70	K	2.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40155e+01
Coeff. B	-3.73043e+03
Coeff. C	-6.51800e+01
Temperature range (K), min.	336.92
Temperature range (K), max.	493.77

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/ci990307l>

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=C24443150&Units=SI>

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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