

Butane, 1,2-dibromo-3-methyl-

Other names:	1,2-Dibromo-3-methylbutane
Inchi:	InChI=1S/C5H10Br2/c1-4(2)5(7)3-6/h4-5H,3H2,1-2H3
InchiKey:	XCVOFNNXLRFMGX-UHFFFAOYSA-N
Formula:	C5H10Br2
SMILES:	CC(C)C(Br)CBr
Mol. weight [g/mol]:	229.94
CAS:	10288-13-8

Physical Properties

Property code	Value	Unit	Source
gf	14.98	kJ/mol	Joback Method
hf	-104.43	kJ/mol	Joback Method
hfus	12.23	kJ/mol	Joback Method
hvap	38.82	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	2.801		Crippen Method
mcvol	116.310	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
tb	445.24	K	Joback Method
tc	659.19	K	Joback Method
tf	235.71	K	Joback Method
vc	0.427	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.24	J/mol×K	445.24	Joback Method
cpg	204.99	J/mol×K	480.90	Joback Method
cpg	214.15	J/mol×K	516.56	Joback Method
cpg	222.76	J/mol×K	552.22	Joback Method
cpg	230.84	J/mol×K	587.88	Joback Method
cpg	238.42	J/mol×K	623.54	Joback Method
cpg	245.55	J/mol×K	659.19	Joback Method
dvisc	0.0063998	Paxs	235.71	Joback Method

dvisc	0.0029311	Paxs	270.63	Joback Method
dvisc	0.0016048	Paxs	305.55	Joback Method
dvisc	0.0009942	Paxs	340.48	Joback Method
dvisc	0.0006733	Paxs	375.40	Joback Method
dvisc	0.0004872	Paxs	410.32	Joback Method
dvisc	0.0003710	Paxs	445.24	Joback Method

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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10288138&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/ci9903071
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
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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