

2,3-Dibromo-2,3-dimethylbutane

Other names:	Butane, 2,3-dibromo-2,3-dimethyl-
Inchi:	InChI=1S/C6H12Br2/c1-5(2,7)6(3,4)8/h1-4H3
InchiKey:	KLFWZEFFWWOMIF-UHFFFAOYSA-N
Formula:	C6H12Br2
SMILES:	CC(C)(Br)C(C)(C)Br
Mol. weight [g/mol]:	243.97
CAS:	594-81-0

Physical Properties

Property code	Value	Unit	Source
gf	33.96	kJ/mol	Joback Method
hf	-132.01	kJ/mol	Joback Method
hfus	7.04	kJ/mol	Joback Method
hvap	39.23	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.333		Crippen Method
mcvol	130.400	ml/mol	McGowan Method
pc	3819.82	kPa	Joback Method
rinpol	1054.00		NIST Webbook
rinpol	1054.00		NIST Webbook
tb	462.54	K	Joback Method
tc	692.70	K	Joback Method
tf	435.15 ± 3.00	K	NIST Webbook
vc	0.473	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	240.16	J/molxK	462.54	Joback Method
cpg	293.45	J/molxK	654.34	Joback Method
cpg	284.66	J/molxK	615.98	Joback Method
cpg	275.03	J/molxK	577.62	Joback Method
cpg	264.46	J/molxK	539.26	Joback Method
cpg	252.87	J/molxK	500.90	Joback Method

cpg	301.49	J/mol×K	692.70	Joback Method
dvisc	0.0003786	Paxs	462.54	Joback Method
dvisc	0.0005061	Paxs	432.42	Joback Method
dvisc	0.0007064	Paxs	402.30	Joback Method
dvisc	0.0010406	Paxs	372.18	Joback Method
dvisc	0.0016413	Paxs	342.06	Joback Method
dvisc	0.0028269	Paxs	311.94	Joback Method
dvisc	0.0054690	Paxs	281.82	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.43897e+01
Coeff. B	-3.97648e+03
Coeff. C	-7.35200e+01
Temperature range (K), min.	355.50
Temperature range (K), max.	511.54

Sources

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=C594810&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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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