

Propane, 1,3-dibromo-2-methyl-

Other names:	1,3-Dibromoisobutane
Inchi:	InChI=1S/C4H8Br2/c1-4(2-5)3-6/h4H,2-3H2,1H3
InchiKey:	SMGXHVWYXQYMNN-UHFFFAOYSA-N
Formula:	C4H8Br2
SMILES:	CC(CBr)CBr
Mol. weight [g/mol]:	215.91
CAS:	28148-04-1

Physical Properties

Property code	Value	Unit	Source
gf	9.00	kJ/mol	Joback Method
hf	-78.51	kJ/mol	Joback Method
hfl	-141.80	kJ/mol	NIST Webbook
hfus	13.16	kJ/mol	Joback Method
hvap	36.98	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.412		Crippen Method
mcvol	102.220	ml/mol	McGowan Method
pc	4717.12	kPa	Joback Method
rinpol	903.00		NIST Webbook
tb	422.80	K	Joback Method
tc	634.29	K	Joback Method
tf	239.44	K	Joback Method
vc	0.378	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	199.46	J/molxK	634.29	Joback Method
cpg	193.62	J/molxK	599.04	Joback Method
cpg	187.39	J/molxK	563.79	Joback Method
cpg	180.76	J/molxK	528.54	Joback Method
cpg	173.70	J/molxK	493.30	Joback Method
cpg	166.17	J/molxK	458.05	Joback Method

cpg	158.15	J/mol×K	422.80	Joback Method
dvisc	0.0043966	Paxs	239.44	Joback Method
dvisc	0.0004216	Paxs	422.80	Joback Method
dvisc	0.0005352	Paxs	392.24	Joback Method
dvisc	0.0007073	Paxs	361.68	Joback Method
dvisc	0.0009841	Paxs	331.12	Joback Method
dvisc	0.0014644	Paxs	300.56	Joback Method
dvisc	0.0023844	Paxs	270.00	Joback Method
hvapt	45.10	kJ/mol	367.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28148041&Units=SI
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

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical 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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