

Ethane, hexabromo-

Other names:	Hexabromoethane
Inchi:	InChI=1S/C2Br6/c3-1(4,5)2(6,7)8
InchiKey:	POJPMDDRCILHJ-UHFFFAOYSA-N
Formula:	C2Br6
SMILES:	BrC(Br)(Br)C(Br)(Br)Br
Mol. weight [g/mol]:	503.44
CAS:	594-73-0

Physical Properties

Property code	Value	Unit	Source
gf	57.56	kJ/mol	Joback Method
hf	133.00	kJ/mol	NIST Webbook
hfus	17.82	kJ/mol	Joback Method
hvap	56.06	kJ/mol	Joback Method
log10ws	-5.45		Crippen Method
logp	4.663		Crippen Method
mcvol	144.040	ml/mol	McGowan Method
pc	10896.05	kPa	Joback Method
tb	635.66	K	Joback Method
tc	955.52	K	Joback Method
tf	475.94	K	Joback Method
vc	0.497	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.53	J/molxK	635.66	Joback Method
cpg	177.43	J/molxK	902.21	Joback Method
cpg	177.20	J/molxK	848.90	Joback Method
cpg	177.32	J/molxK	795.59	Joback Method
cpg	177.46	J/molxK	742.28	Joback Method
cpg	177.31	J/molxK	688.97	Joback Method
cpg	178.35	J/molxK	955.52	Joback Method
dvisc	0.0002329	Paxs	635.66	Joback Method

dvisc	0.0002802	Paxs	609.04	Joback Method
dvisc	0.0003428	Paxs	582.42	Joback Method
dvisc	0.0004276	Paxs	555.80	Joback Method
dvisc	0.0005454	Paxs	529.18	Joback Method
dvisc	0.0007138	Paxs	502.56	Joback Method
dvisc	0.0009628	Paxs	475.94	Joback Method

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=C594730&Units=SI
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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